

## Supporting Information

# Mechanistic insights of electrocatalytic CO<sub>2</sub> reduction by Mn complexes: synergistic effects of the ligands

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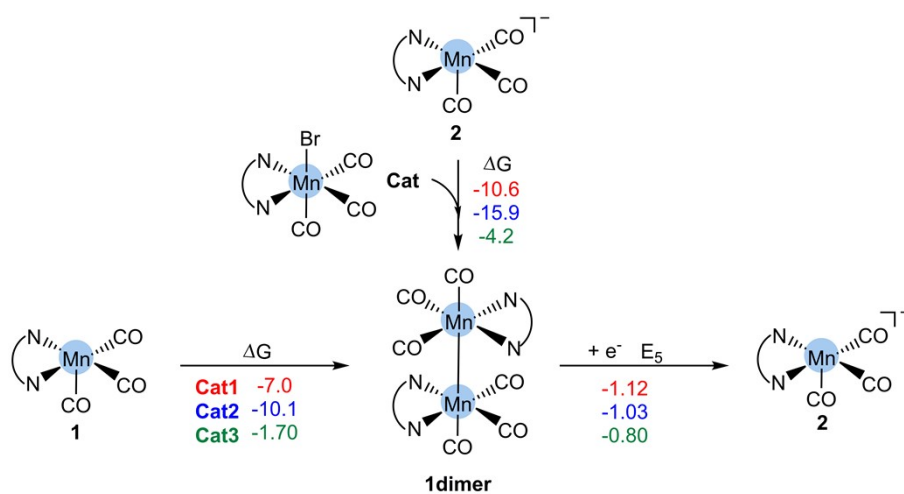
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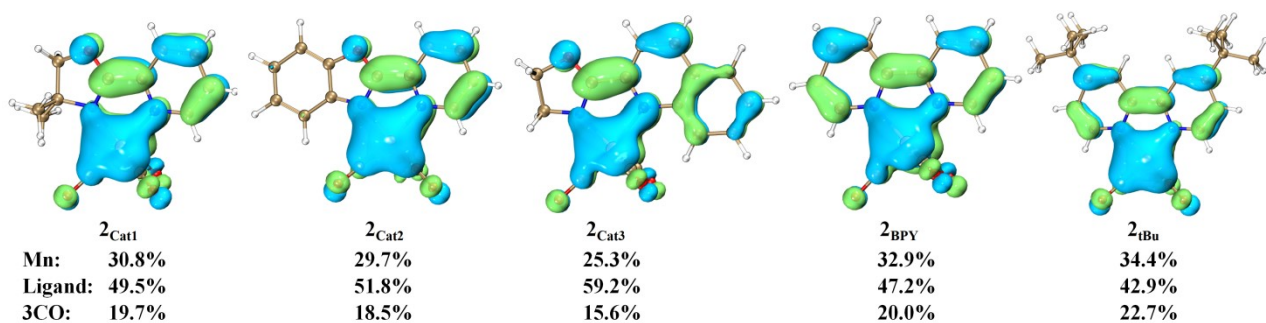
<sup>‡</sup>These authors contributed equally to this work.

**Table S1.** Experimentally obtained and calculated carbonyl stretching vibration frequencies,  $\nu_{\text{CO}}$  ( $\text{cm}^{-1}$ ) of Mn complexes. The calculated values of  $\nu_{\text{CO}}$  have been scaled by 0.965.

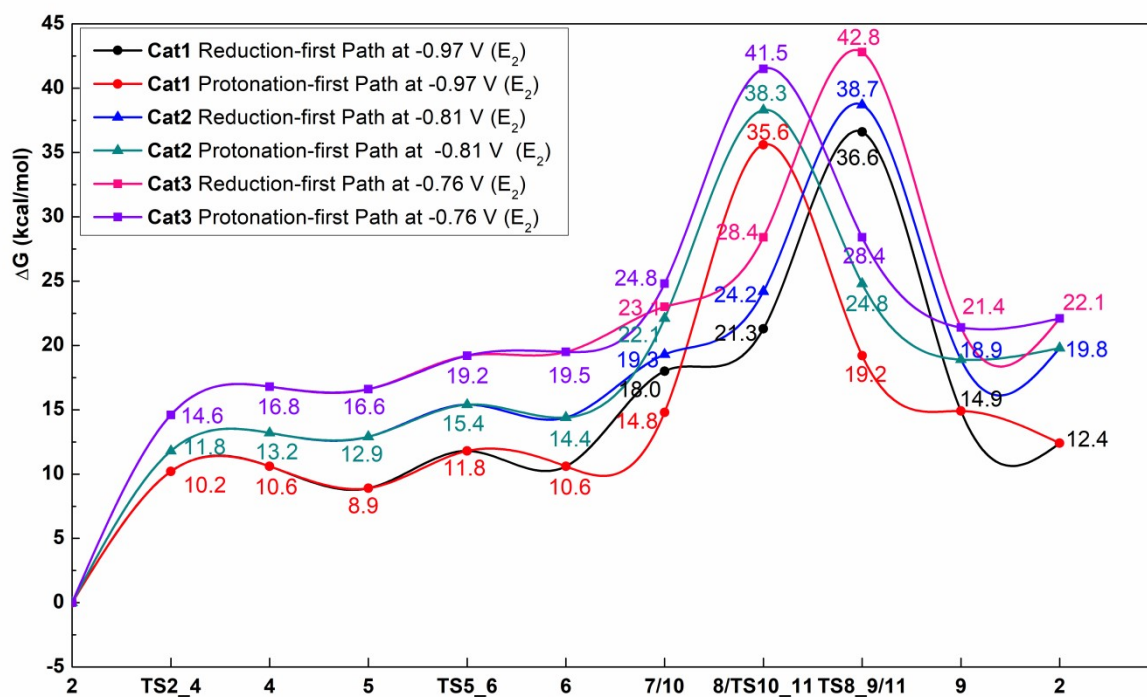
Species	Calcd	Exptl
<b>Cat1</b> Mn(pyrox)(CO) <sub>3</sub> Br	2027, 1969, 1948	2028, 1932, 1923
<b>1dimer</b> <sub>Cat1</sub> [Mn(pyrox)(CO) <sub>3</sub> ] <sub>2</sub>	1981, 1947, 1925, 1903, 1886, 1881	1967, 1929, 1881, 1855
<b>2</b> <sub>Cat1</sub> [Mn(pyrox)(CO) <sub>3</sub> ] <sup>-</sup>	1915, 1849, 1839	1911, 1806
<b>14</b> <sub>Cat1</sub> [Mn(pyrox)(CO) <sub>3</sub> (HCO <sub>3</sub> ) ]	2037, 1975, 1949, 1683, 1649	2037, 1940, 1914, 1689



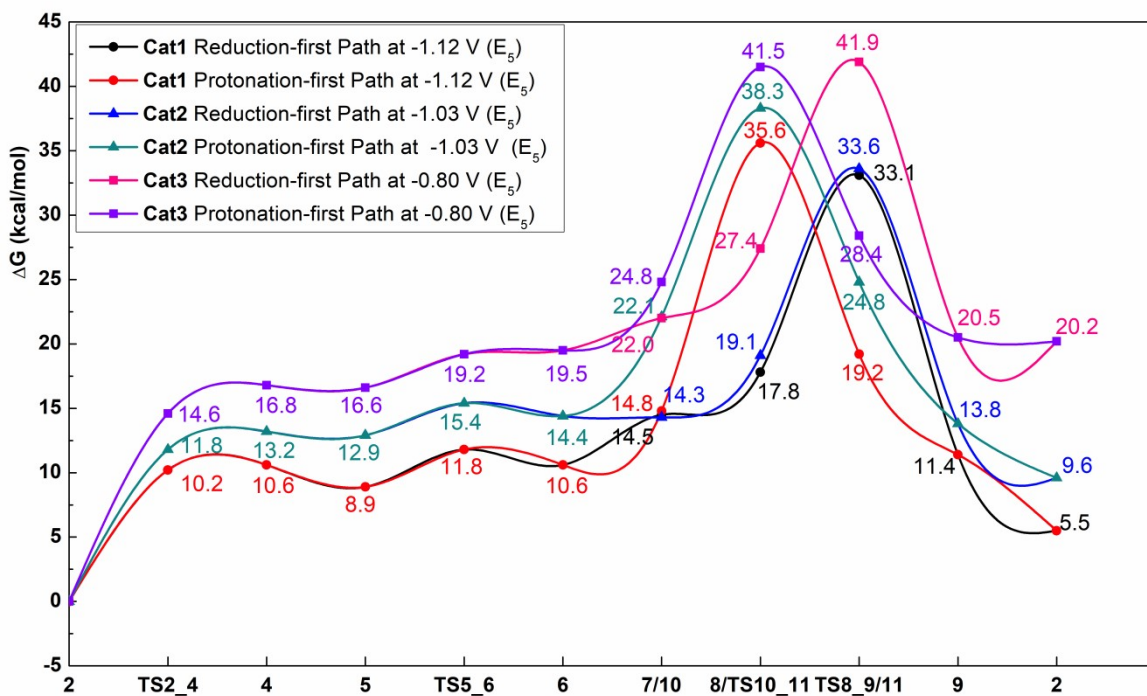
**Figure S1.** Gibbs free energies (kcal/mol) of **1dimer** formations and their reduction potentials (V vs. NHE).



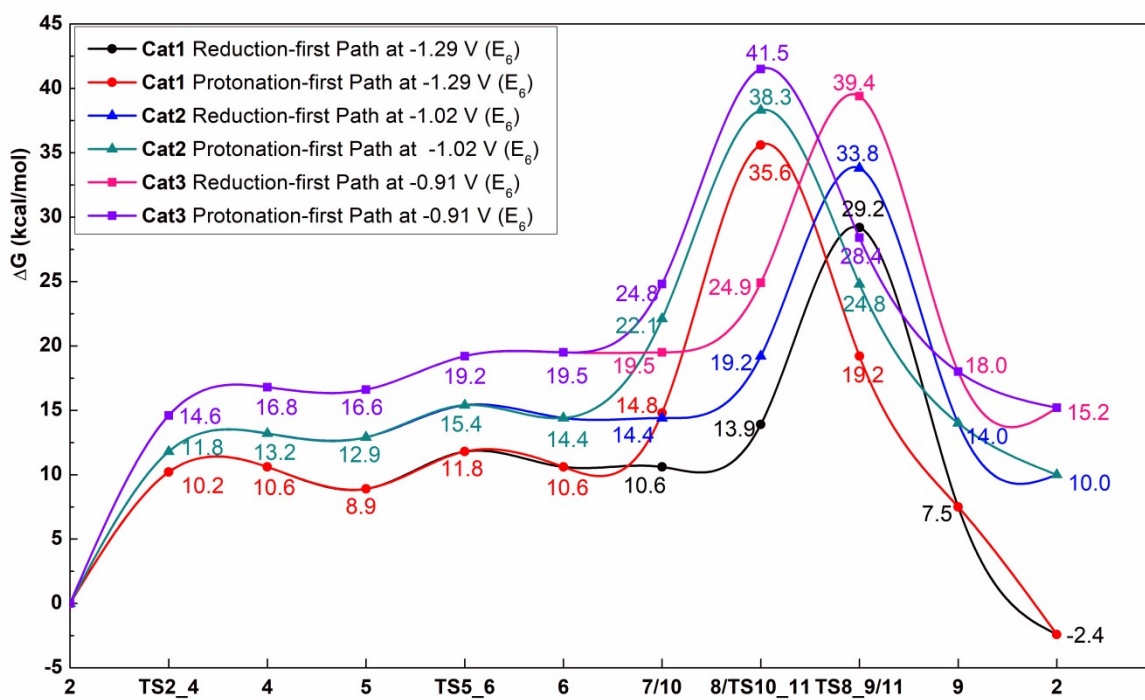
**Figure S2.** Plots of the highest occupied molecular orbitals (HOMO) of the active catalysts **2** together with orbital contributions of Mn atoms.



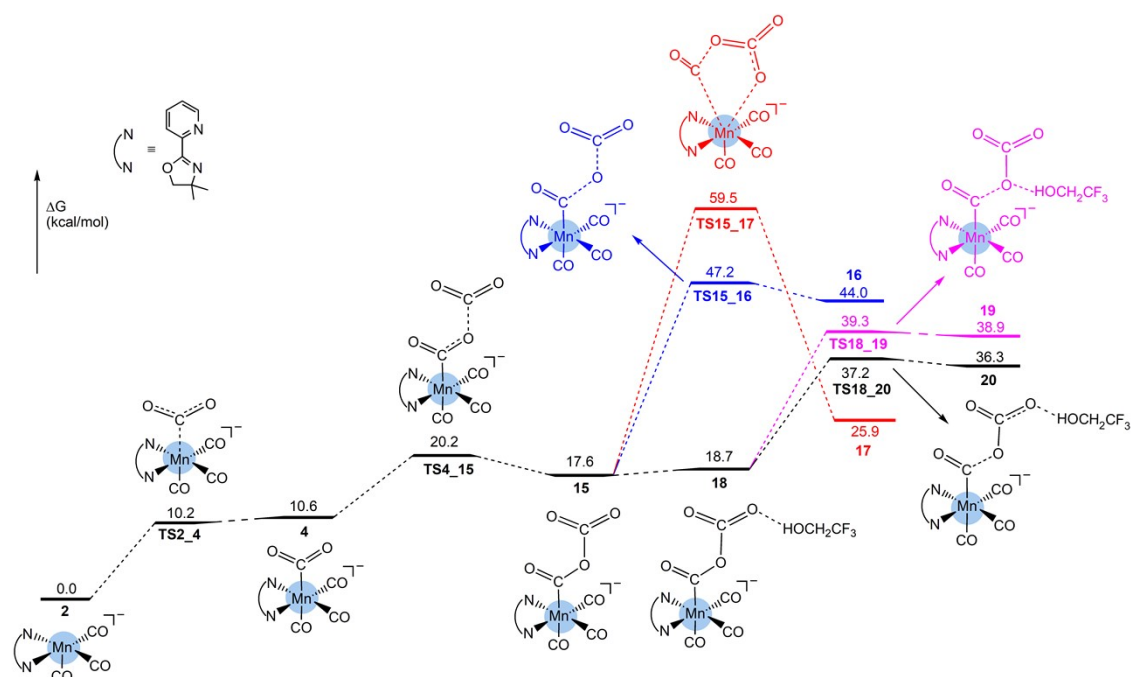
**Figure S3.** The free energy profiles for catalytic reduction of  $\text{CO}_2$  to  $\text{CO}$  when  $E_2$  was set as controlled potential.



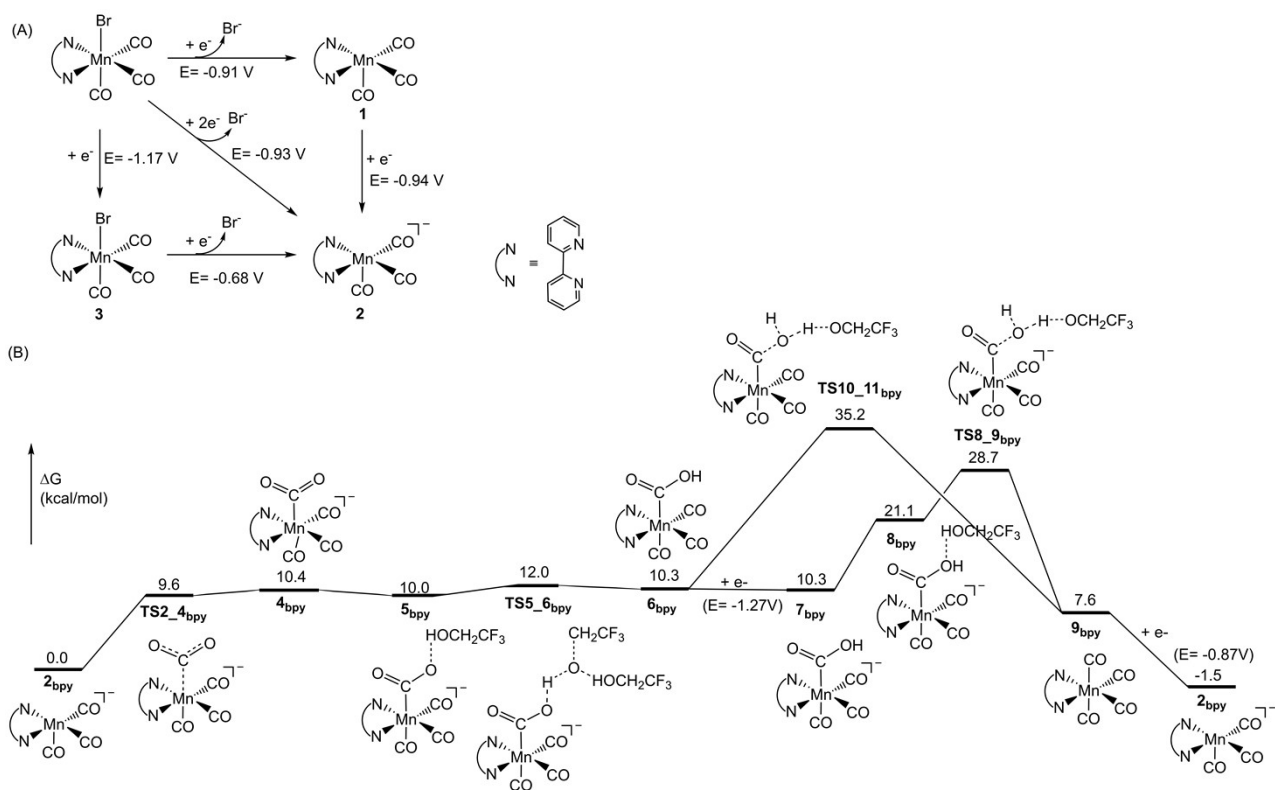
**Figure S4.** The free energy profiles for catalytic reduction of CO<sub>2</sub> to CO when E<sub>5</sub> was set as controlled potential.



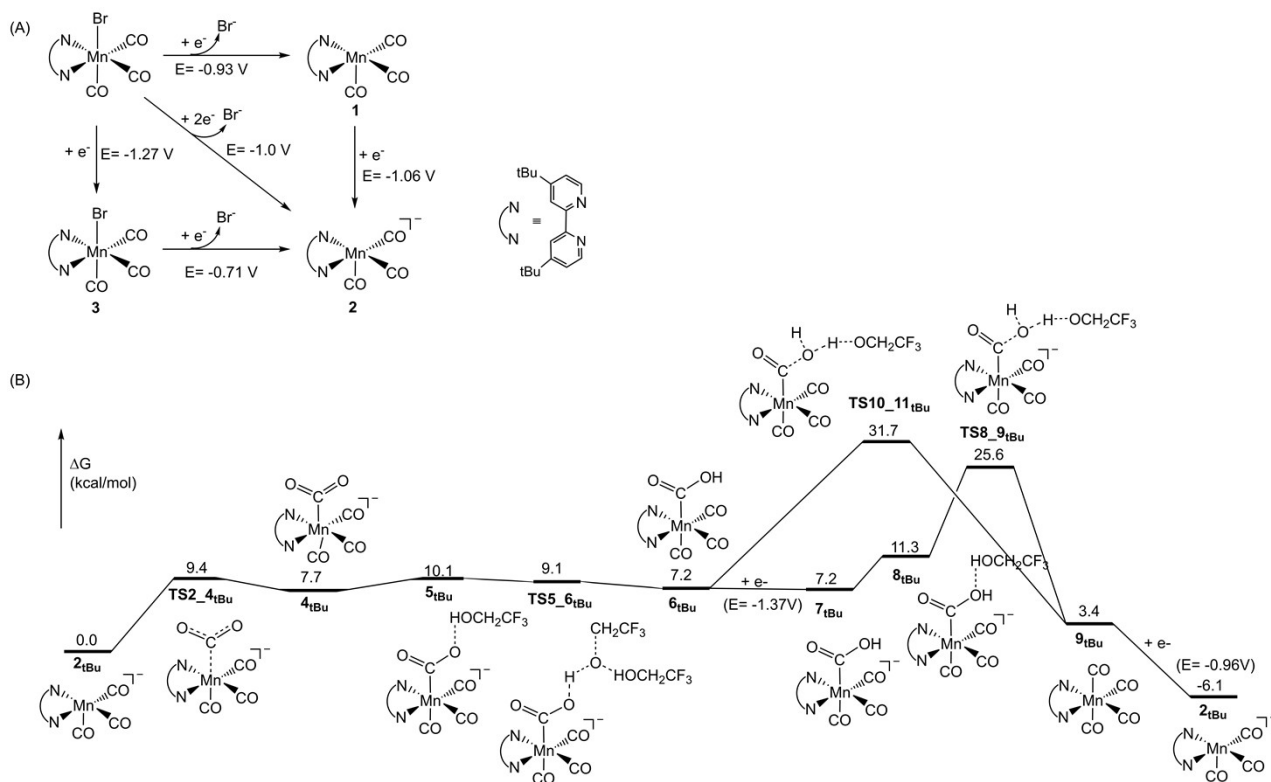
**Figure S5.** The free energy profiles for catalytic reduction of CO<sub>2</sub> to CO when E<sub>6</sub> was set as controlled potential.



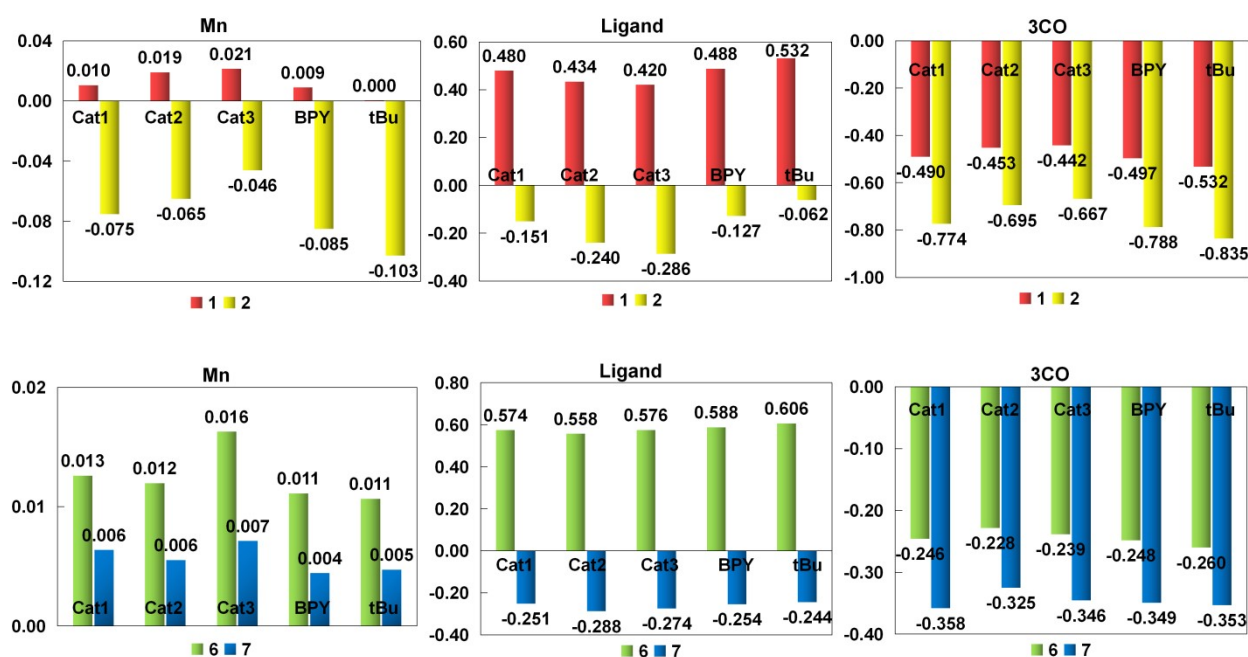
**Figure S6.** Calculated free energy profiles of the possible paths for the reaction of complex **2** with the second CO<sub>2</sub> molecule



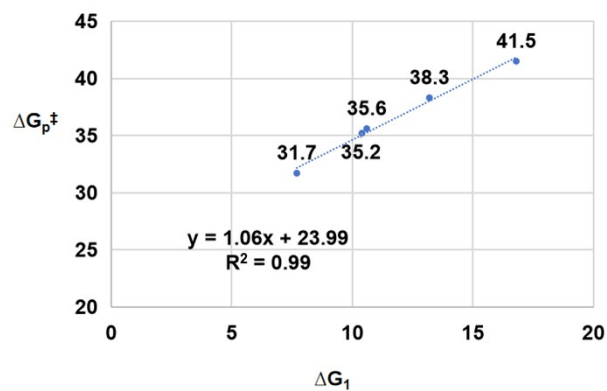
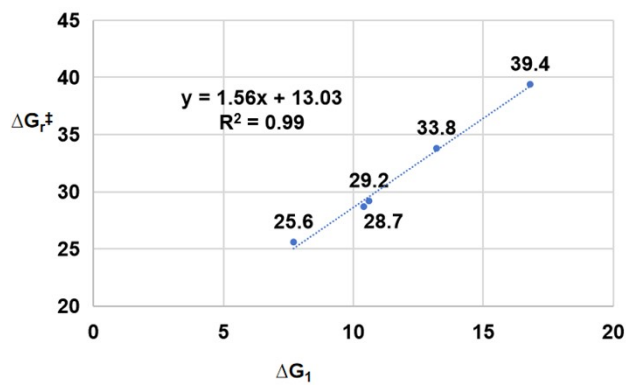
**Figure S7.** The free energy profile of **BPY** mediated CO<sub>2</sub> reduction under E<sub>6</sub> (-1.27 V).



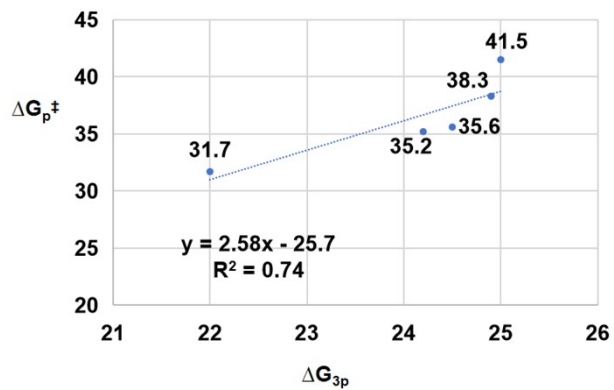
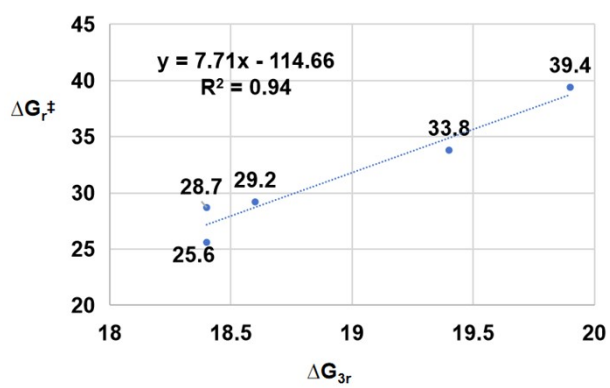
**Figure S8.** The free energy profile of  $2_{tBu}$  mediated  $CO_2$  reduction under  $E_6$  (-1.37 V).



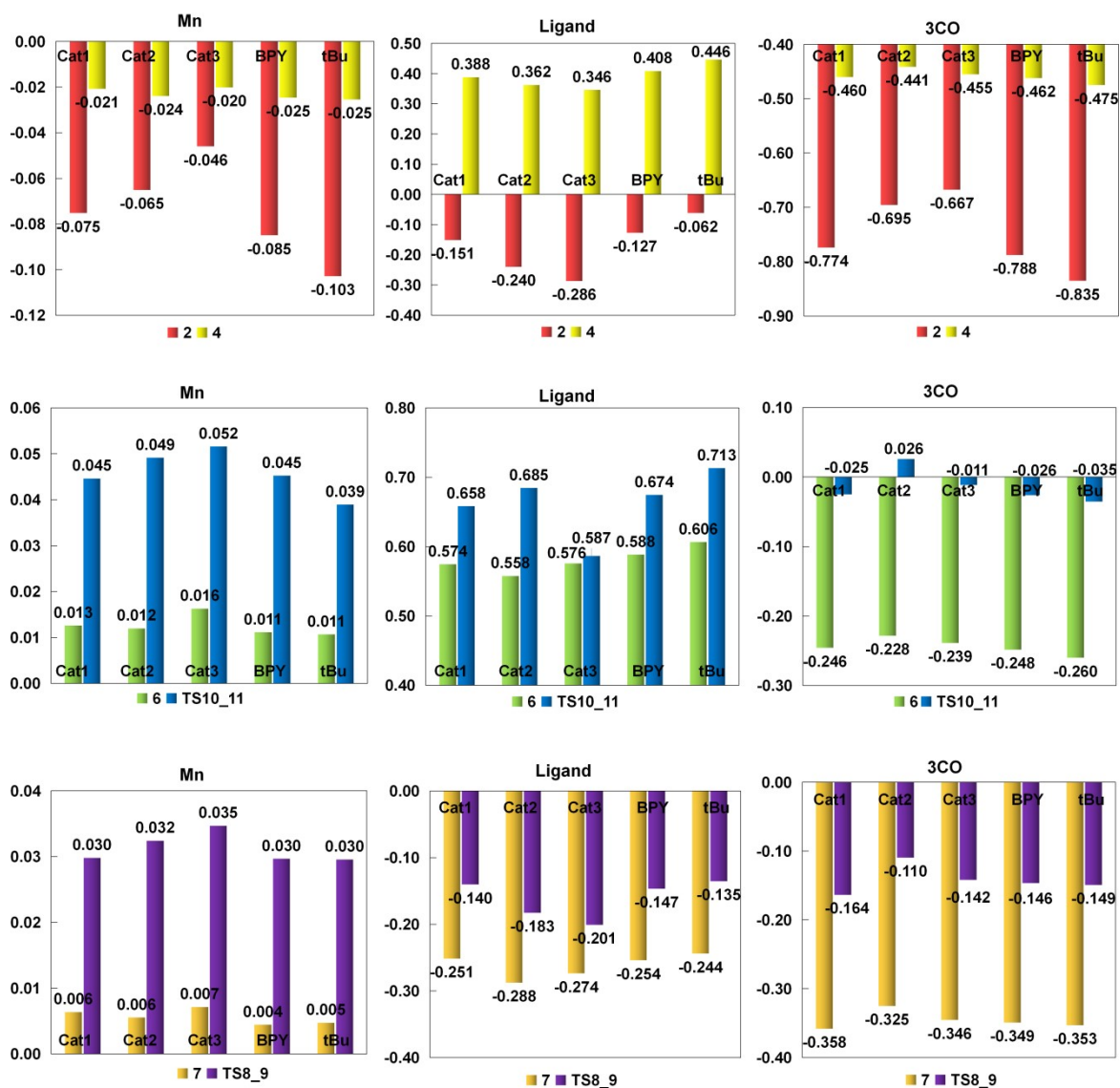
**Figure S9.** The Hirshfeld charges of Mn, heterocyclic ligand and three CO ligands for the two ligand-based reductions ( $1 \rightarrow 2$  and  $6 \rightarrow 7$ ).



**Figure S10.** Linear relationships of  $\Delta G_{r}^{\ddagger}/\Delta G_1$  and  $\Delta G_{p}^{\ddagger}/\Delta G_1$ .

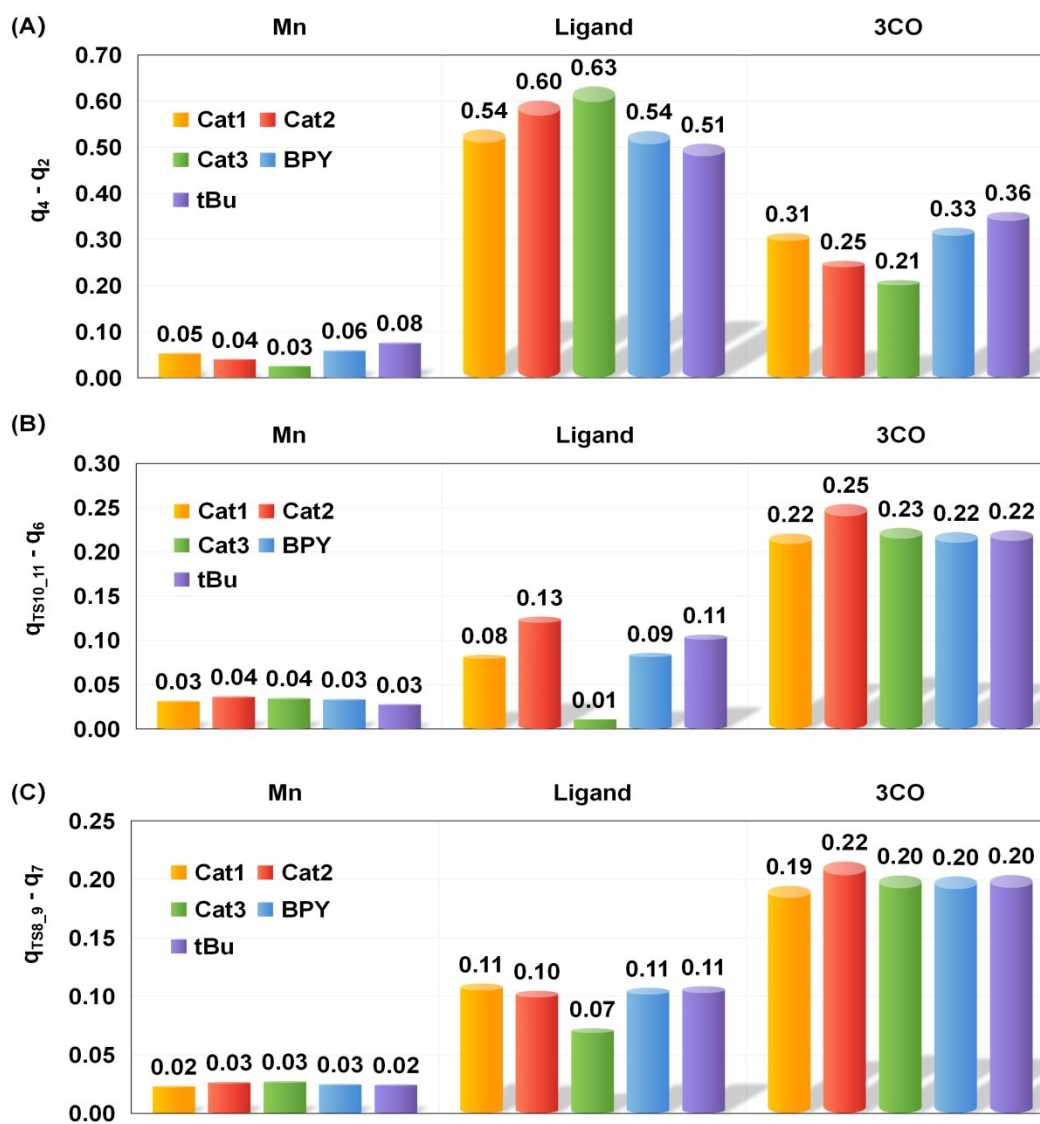


**Figure S11.** Linear relationships of  $\Delta G_{r}^{\ddagger}/\Delta G_{3r}$  and  $\Delta G_{p}^{\ddagger}/\Delta G_{3p}$ .

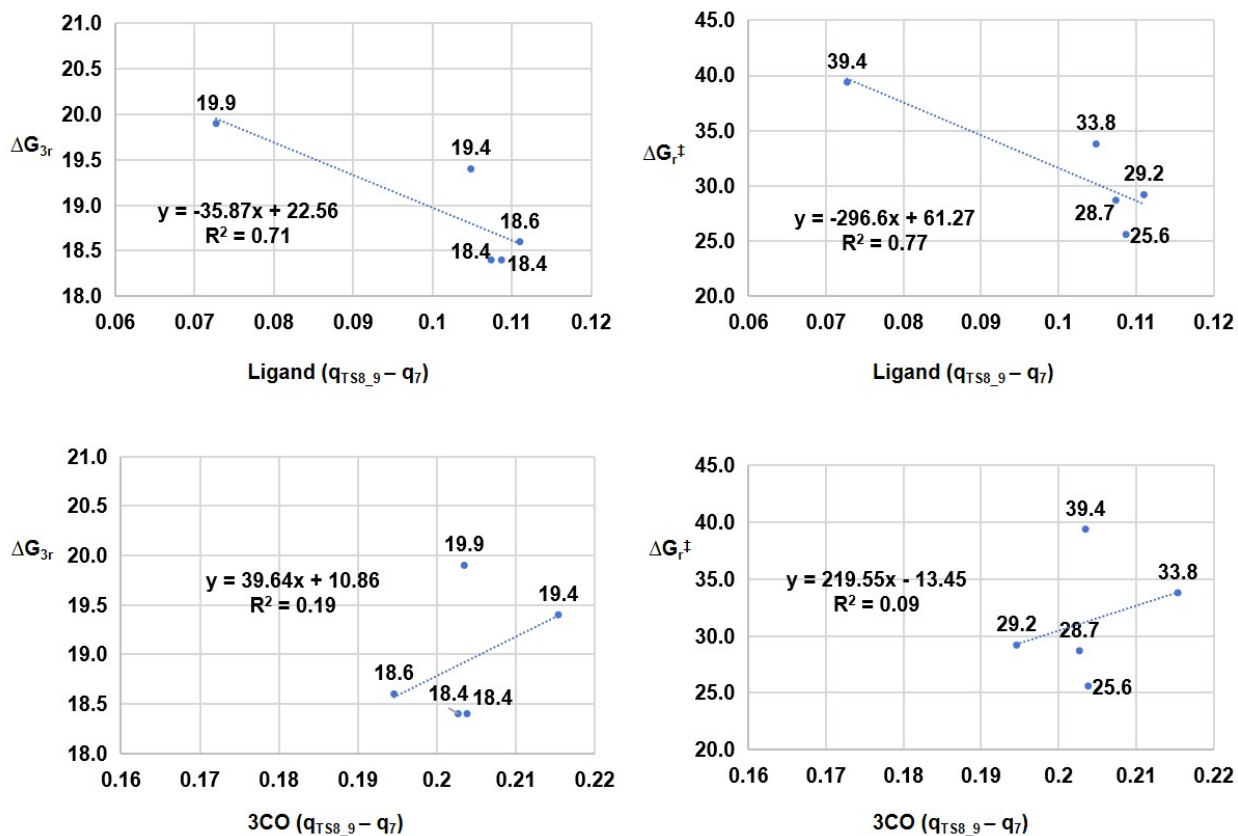


**Figure S12.** The Hirshfeld charges of Mn, heterocyclic ligand and three CO ligands for CO<sub>2</sub> activation (2→4) and C-O break (6→TS10\_11 and 7→TS8\_9).

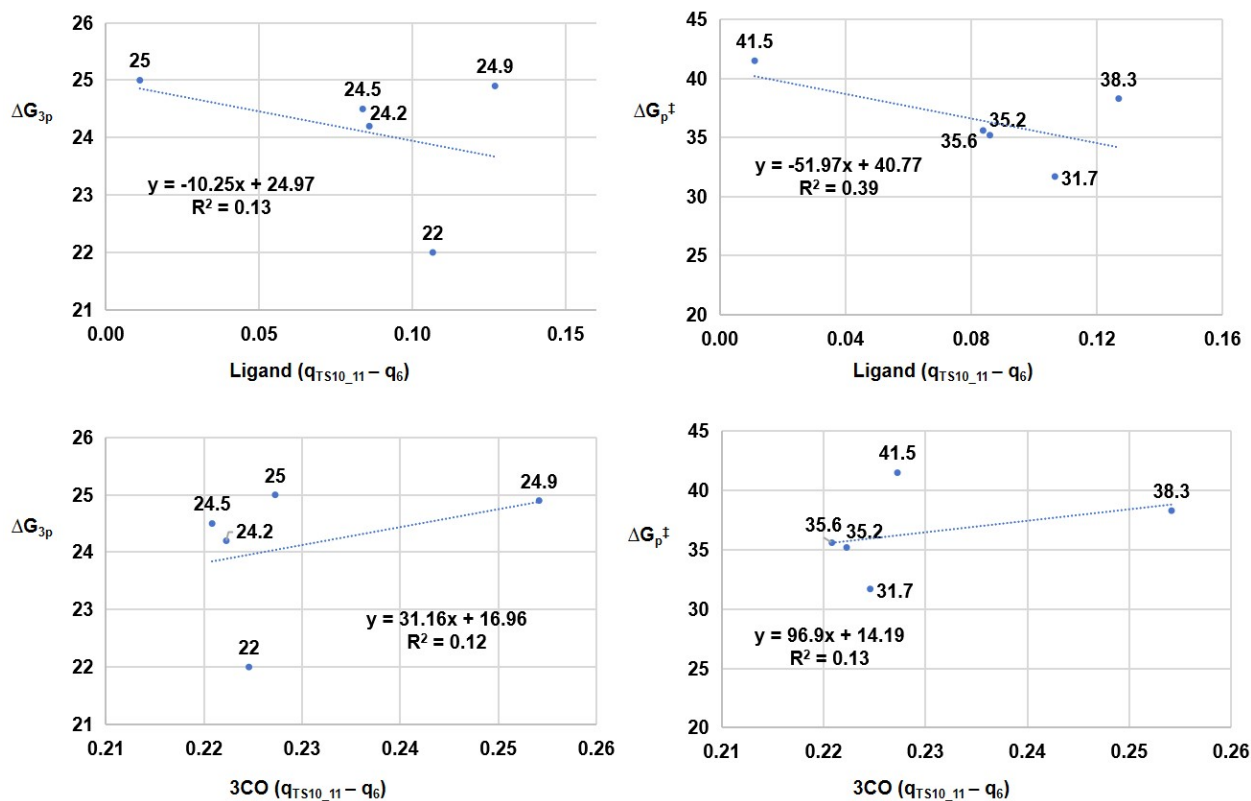




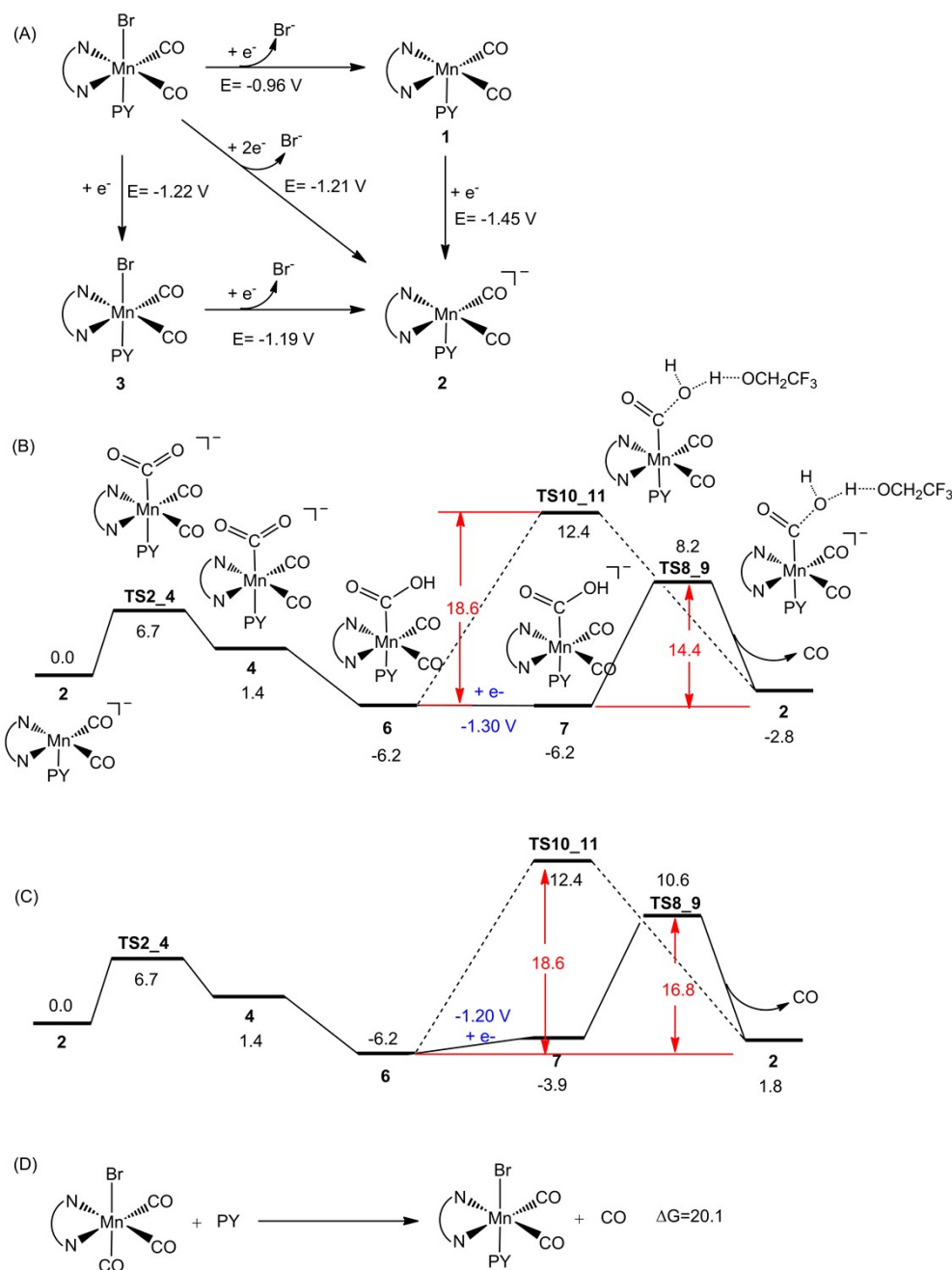
**Figure S13.** The changes of Hirshfeld charge of Mn, heterocyclic ligand and three CO ligands for  $\text{CO}_2$  activation  $2 \rightarrow 4$  (A) and C-O break  $6 \rightarrow \text{TS10\_11}$  (B) and  $7 \rightarrow \text{TS8\_9}$  (C).



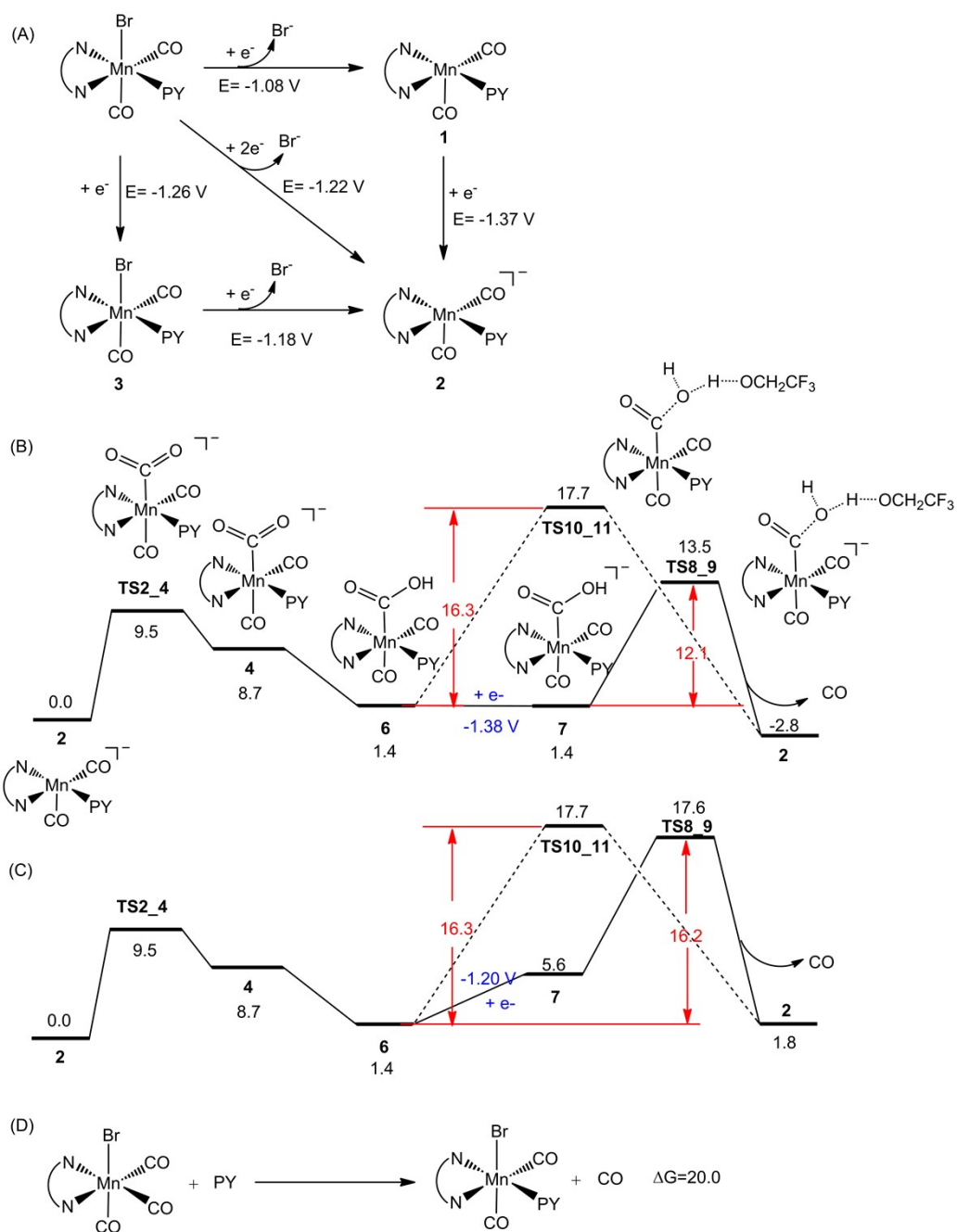
**Figure S14.** Linear relationships between  $\Delta G_{3r}/\Delta G_{r^\ddagger}$  and the transferred charges of Ligand/3CO from 7 to TS8\_9.



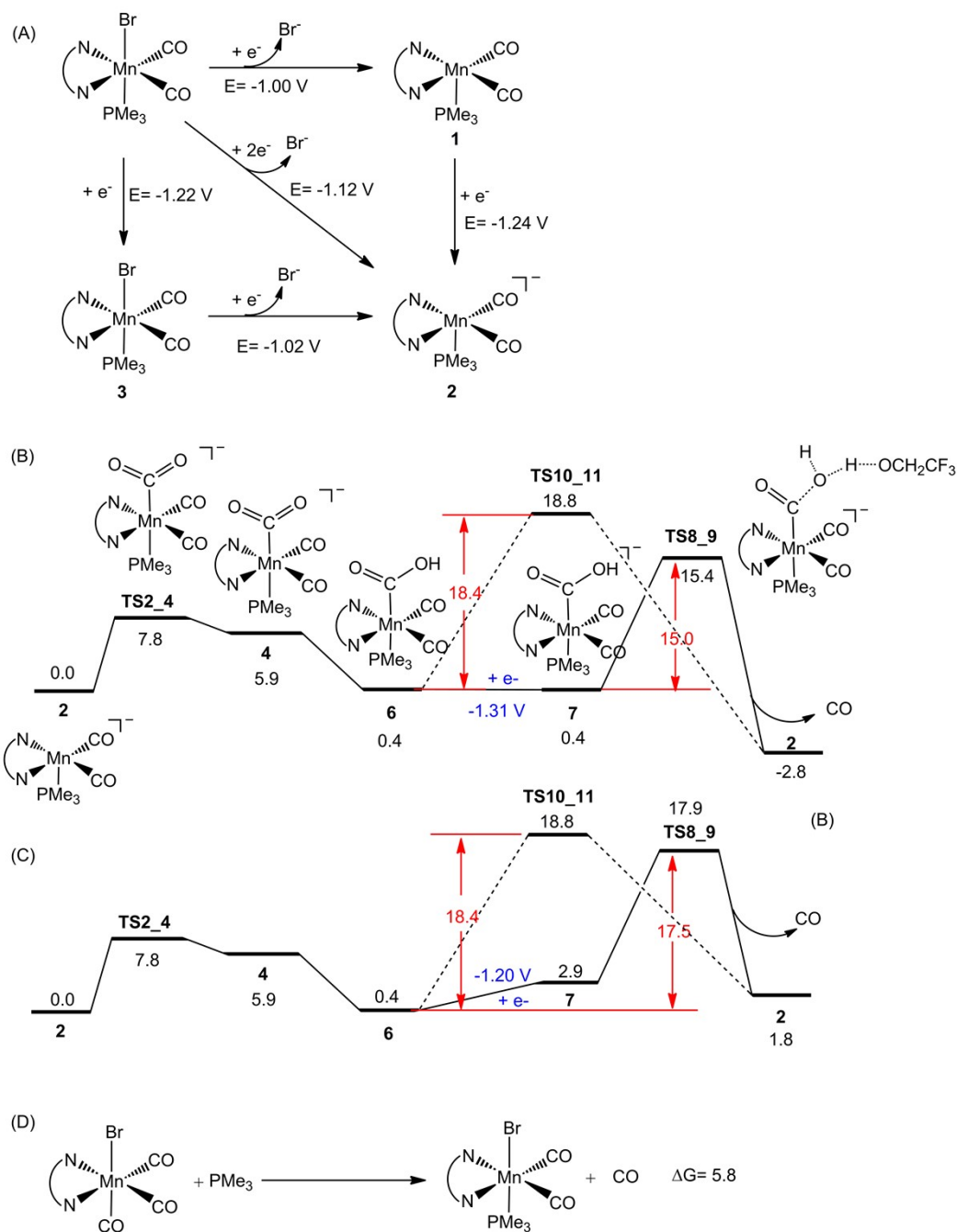
**Figure S15.** Linear relationships between  $\Delta G_{3p}/\Delta G_{p^\ddagger}$  and the transferred charges of Ligand/3CO from **6** to TS10\_11.



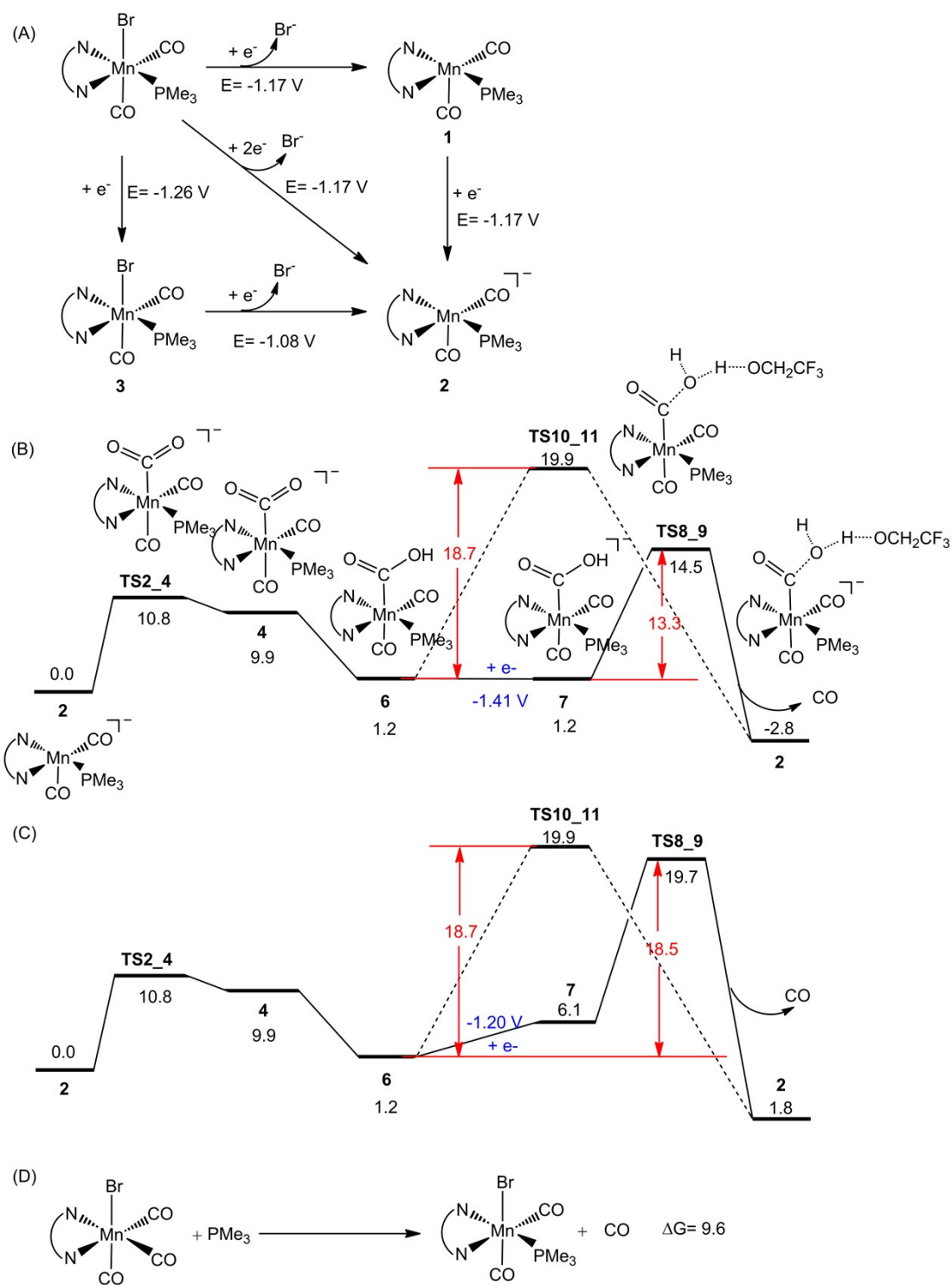
**Figure S16.** The catalytic mechanism of the Mn complex in which the axial CO ligand was replaced by one pyridine ligand. (A) the generation of active catalyst by two electrons reductions; (B) The free energy profile of CO<sub>2</sub> reduction under -1.30 V; (C) The free energy profile of CO<sub>2</sub> reduction under -1.20 V; (D) Thermodynamics for the substitution of axial CO by pyridine.



**Figure S17.** The catalytic mechanism of the Mn complex in which one of the latitudinal CO ligands was replaced by one pyridine ligand. (A) the generation of active catalyst by two electrons reductions; (B) The free energy profile of CO<sub>2</sub> reduction under -1.38 V; (C) The free energy profile of CO<sub>2</sub> reduction under -1.20 V; (D) Thermodynamics for the substitution of latitudinal CO by pyridine.



**Figure S18.** The catalytic mechanism of the Mn complex in which the axial CO ligand was replaced by  $\text{PMe}_3$  ligand. (A) the generation of active catalyst by two electrons reductions; (B) The free energy profile of  $\text{CO}_2$  reduction under  $-1.31$  V; (C) The free energy profile of  $\text{CO}_2$  reduction under  $-1.20$  V; (D) Thermodynamics for the substitution of axial CO by  $\text{PMe}_3$ .



**Figure S19.** The catalytic mechanism of the Mn complex in which one of the latitudinal CO ligands was replaced by  $\text{PMe}_3$ . (A) the generation of active catalyst by two electrons reductions; (B) The free energy profile of  $\text{CO}_2$  reduction under  $-1.41\text{ V}$ ; (C) The free energy profile of  $\text{CO}_2$  reduction under  $-1.20\text{ V}$ ; (D) Thermodynamics for the substitution of latitudinal CO by  $\text{PMe}_3$ .

## Cartesian coordinates of all optimized structures

### CO<sub>2</sub>

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16916900
O	0.00000000	0.00000000	-1.16916900

### CO

C	0.00000000	0.00000000	-0.64984200
O	0.00000000	0.00000000	0.48738200

### H<sub>2</sub>O

O	0.00000000	0.00000000	0.11774000
H	0.00000000	0.76686000	-0.47096100
H	0.00000000	-0.76686000	-0.47096100

### TFE

C	-0.41331700	0.01698100	0.00000900
C	0.91597000	0.74788300	-0.00006200
F	-0.57235800	-0.77492800	1.08850700
F	-1.43693100	0.90942400	-0.00004800
F	-0.57237600	-0.77508800	-1.08837300
O	1.94241800	-0.22671800	-0.00009200
H	2.79732200	0.22479400	0.00044200
H	0.94116700	1.38253200	-0.89324600
H	0.94123800	1.38256200	0.89309500

### TFE-OCH<sub>2</sub>CF<sub>3</sub>

C	2.53358400	-0.33256500	0.01547400
C	1.93745000	0.88117100	0.72093400
F	3.43062000	0.00627700	-0.95031800
F	3.19870000	-1.14009600	0.89324500
F	1.59580100	-1.10901500	-0.59051300
O	1.27508800	1.72324300	-0.15971000
H	0.17247000	1.65522300	-0.02193100
H	1.28203000	0.48021700	1.51007400
H	2.78432000	1.38165700	1.21555700
C	-2.56121600	-0.29443700	-0.01523700
C	-1.79785300	0.82428600	-0.72123400
F	-3.50640900	0.16938900	0.85060300
F	-3.22328100	-1.09631400	-0.90567800
F	-1.75600100	-1.11806700	0.71176100
O	-1.13320000	1.64579500	0.15709300



H	-1.13495400	0.30368500	-1.43948000
H	-2.56563700	1.34661800	-1.32479800

**[Mn(pyrox)(CO)<sub>3</sub>Br]**

**Cat1**

Mn	0.06451100	-0.91461100	0.50252300
N	0.94588100	0.93992600	0.09756700
N	-1.63291300	0.33729100	0.31920000
C	-2.92364700	-0.00407400	0.44451600
C	-3.96447700	0.90987300	0.26254700
C	-3.66209100	2.23047000	-0.06456700
C	-2.32170600	2.59799300	-0.19662500
C	0.08939700	1.87942300	-0.09307300
C	-1.34717400	1.62363000	0.00206900
H	-3.13536100	-1.03549200	0.69916700
H	-4.98990300	0.57747200	0.37816000
H	-4.44993300	2.96135100	-0.21214500
H	-2.02877700	3.61058700	-0.44782600
C	0.14330700	-0.65073500	2.27729800
O	0.18798400	-0.48893700	3.42250900
C	1.59531400	-1.88243500	0.48925400
C	-0.89501500	-2.43844500	0.68759600
O	2.55421400	-2.52799100	0.47769100
O	-1.49849100	-3.41898500	0.79437800
Br	-0.10801500	-1.30164600	-2.07724800
O	0.53703800	3.10952600	-0.36800600
C	1.99345900	2.99340000	-0.45408600
C	2.31371500	1.53491700	0.00223000
H	2.27101000	3.18351400	-1.49328200
H	2.42244400	3.75830200	0.19434000
C	3.16827100	0.80792000	-1.04233100
H	4.11080800	1.34870100	-1.17850500
H	3.40747800	-0.20810400	-0.72207500
H	2.65113400	0.75755500	-2.00375900
C	2.97958000	1.50494900	1.38653200
H	3.11951400	0.47608600	1.72902900
H	3.96348300	1.98235500	1.33348600
H	2.37553000	2.03981100	2.12594200

**1**

Mn	-0.11468700	1.12242800	-0.08722900
N	-0.89406700	-0.77499500	-0.05999500
N	1.62081200	-0.04302700	-0.09932900

C	2.89955900	0.38240800	-0.08842600
C	3.98502600	-0.48927600	-0.06206100
C	3.75659700	-1.87053800	-0.04112100
C	2.44218200	-2.32886500	-0.04143700
C	-0.00280100	-1.71666600	-0.05407800
C	1.40908600	-1.38893600	-0.07051200
H	3.04905200	1.45557900	-0.10097700
H	4.99120400	-0.08529300	-0.05932100
H	4.58509000	-2.57053700	-0.02163900
H	2.20561500	-3.38646800	-0.01800100
C	0.03633400	1.73368700	1.59063800
O	0.13736900	2.16899300	2.67021500
C	-1.67841700	1.95196500	-0.36965700
C	0.70493400	2.50269200	-0.88737400
O	-2.68078100	2.52773700	-0.54012500
O	1.23451700	3.41230500	-1.39739000
O	-0.42207200	-2.99069100	-0.02241800
C	-1.87381700	-2.92854600	0.13528300
C	-2.24043400	-1.42518800	-0.06056300
H	-2.31512500	-3.58688200	-0.61401500
H	-2.10650000	-3.29567200	1.13811800
C	-2.92411600	-1.19043200	-1.41691000
H	-3.88789600	-1.70997300	-1.44028900
H	-3.10390600	-0.12606800	-1.58457500
H	-2.30587200	-1.57163100	-2.23582300
C	-3.10051500	-0.90775300	1.09805500
H	-3.35336800	0.14606800	0.96014100
H	-4.03480300	-1.47725300	1.14654600
H	-2.57749200	-1.02047200	2.05253300

## 2

Mn	-0.11061500	1.09930400	-0.00194900
N	-0.89405500	-0.73777600	0.00620900
N	1.56529200	-0.05311500	-0.04057500
C	2.86338500	0.36326700	-0.03847800
C	3.94598200	-0.49123100	-0.03773200
C	3.72497900	-1.89952400	-0.03085400
C	2.42841300	-2.36080000	-0.02227700
C	-0.01238000	-1.73148300	-0.01061300
C	1.35522000	-1.43088500	-0.02645100
H	3.00611300	1.43921900	-0.03755700
H	4.95057600	-0.08134100	-0.04168400
H	4.56220500	-2.59073900	-0.02839100
H	2.20159900	-3.42237900	-0.01060200

C	0.29688700	1.94895900	1.48038400
O	0.58536100	2.59089100	2.42942100
C	-1.67721300	1.92908200	-0.17805500
C	0.58455700	2.22558100	-1.17155000
O	-2.68733400	2.51989400	-0.30806600
O	1.05828500	3.00672700	-1.91983400
O	-0.52233900	-3.00795400	-0.02774200
C	-1.92201800	-2.85033900	0.30142000
C	-2.25070100	-1.36572800	-0.01671100
H	-2.49543200	-3.56386100	-0.29355000
H	-2.05250200	-3.07147200	1.36800200
C	-2.86449200	-1.22155200	-1.42132900
H	-3.84461800	-1.71064100	-1.45914000
H	-2.99263400	-0.16694600	-1.67821900
H	-2.21894400	-1.68374700	-2.17571500
C	-3.18214400	-0.78626800	1.05352300
H	-3.45635400	0.24593200	0.82831400
H	-4.10391000	-1.37777900	1.10225000
H	-2.70401300	-0.81353300	2.03770000

### 3

Mn	-0.01162900	-0.81356300	0.60986400
N	1.06528400	0.80813300	-0.06380400
N	-1.54593900	0.54870100	0.30952900
C	-2.87057100	0.40017200	0.51962500
C	-3.80811000	1.39694800	0.29582900
C	-3.36209000	2.66565300	-0.18010700
C	-2.01565900	2.85612400	-0.39794300
C	0.29147700	1.85382500	-0.30366000
C	-1.10727000	1.79254800	-0.15176600
H	-3.18997300	-0.57150300	0.88348300
H	-4.85788900	1.19844400	0.48151700
H	-4.07128700	3.46687200	-0.36467100
H	-1.62773600	3.80473700	-0.75557700
C	0.14473300	-0.38050400	2.31707900
O	0.22795800	-0.08161400	3.43790900
C	1.38491400	-1.95727300	0.65758400
C	-1.13945000	-2.17633800	0.96173900
O	2.25547000	-2.72382200	0.70914500
O	-1.85489500	-3.05958200	1.19946800
Br	-0.37860500	-1.65154100	-2.07355900
O	0.93647200	3.00532100	-0.66217700
C	2.31838500	2.61940000	-0.87130700
C	2.47633700	1.26906800	-0.12242500

H	2.48129500	2.50627000	-1.94950400
H	2.95526300	3.41644300	-0.48333900
C	3.38393300	0.31922400	-0.91242800
H	4.37200900	0.77445700	-1.04610500
H	3.52383000	-0.62720600	-0.38554400
H	2.96522600	0.10925200	-1.90062300
C	3.02635400	1.48174200	1.30151400
H	3.02971500	0.53868800	1.85579300
H	4.05436300	1.85996700	1.26240900
H	2.41373100	2.20279400	1.85288200

**1dimer**

Mn	1.19855600	-0.35531700	1.07673900
O	2.56164300	-0.32876700	3.66817900
O	-1.25714300	0.55018200	2.45322000
O	0.53911300	-3.20599800	1.52091400
N	1.80276500	1.57854700	0.60502100
N	2.85131700	-0.71412100	-0.11782900
C	2.05653000	-0.33808100	2.61531600
C	-0.34290600	0.17561100	1.82609900
C	0.76534900	-2.08480700	1.29571100
C	1.27304000	2.74026600	1.04540900
H	0.38394500	2.66206300	1.65861600
C	1.82068500	3.98391700	0.75122700
H	1.34444300	4.87753100	1.13925300
C	2.97658700	4.05940100	-0.03869400
C	3.54252000	2.87546500	-0.49697500
H	4.44042900	2.86875400	-1.10443800
C	2.93556800	1.66259300	-0.15382000
C	3.45303400	0.36309700	-0.51070300
Mn	-1.19855100	-0.35530600	-1.07673900
O	-2.56162300	-0.32887500	-3.66818600
O	1.25714500	0.55017900	-2.45323200
O	-0.53907400	-3.20598500	-1.52088800
N	-1.80278800	1.57854700	-0.60502400
N	-2.85130800	-0.71413500	0.11782800
C	-2.05652900	-0.33807600	-2.61531300
C	0.34289800	0.17566000	-1.82609700
C	-0.76530600	-2.08478800	-1.29571300
C	-1.27308100	2.74027400	-1.04541400
H	-0.38398700	2.66208300	-1.65862300
C	-1.82074300	3.98391700	-0.75123100
H	-1.34451400	4.87753800	-1.13925800
C	-2.97664300	4.05938500	0.03869400

C	-3.54255700	2.87544100	0.49697800
H	-4.44046600	2.86871700	1.10444300
C	-2.93559100	1.66257700	0.15382000
C	-3.45303800	0.36307500	0.51070300
H	-3.42205200	5.01784500	0.28335700
H	3.42198300	5.01786700	-0.28335600
O	4.60316700	0.23778900	-1.20286300
C	3.70829600	-1.87526900	-0.51371300
C	4.76892100	-1.19242600	-1.42835000
H	4.58914100	-1.38096100	-2.49051100
H	5.79743100	-1.45275100	-1.17411300
C	4.35619600	-2.48324300	0.74158000
H	3.59707700	-2.89152400	1.41343400
H	5.03134700	-3.29570700	0.45222700
H	4.93488000	-1.73124600	1.28734800
C	2.91865600	-2.93079000	-1.29352800
H	3.60491100	-3.70071700	-1.66319500
H	2.17299600	-3.41682700	-0.66257400
H	2.41034300	-2.48365700	-2.15201300
O	-4.60317000	0.23775200	1.20286400
C	-4.76890600	-1.19246600	1.42834900
C	-3.70827300	-1.87529500	0.51371100
H	-4.58912100	-1.38100000	2.49050900
H	-5.79741300	-1.45280300	1.17411300
C	-2.91862300	-2.93080800	1.29352700
H	-3.60487200	-3.70074000	1.66319500
H	-2.17295900	-3.41684000	0.66257700
H	-2.41031500	-2.48366900	2.15201200
C	-4.35616700	-2.48327700	-0.74158200
H	-3.59704400	-2.89155000	-1.41343600
H	-5.03131000	-3.29574700	-0.45222900
H	-4.93485900	-1.73128600	-1.28735100

#### TS2\_4

Mn	-0.16842900	-0.98548700	-0.46025000
N	-0.78624800	0.91669400	-0.20933800
N	1.60947900	-0.01871900	-0.26607500
C	2.86724400	-0.53757700	-0.34221900
C	4.01912800	0.21527200	-0.23004700
C	3.92207600	1.61861000	-0.03460800
C	2.66495100	2.18261300	0.03062100
C	0.18271600	1.79103200	-0.06111800
C	1.52543700	1.35362800	-0.08496200
H	2.92578300	-1.60917900	-0.49858100

H	4.98416200	-0.27664300	-0.29377400
H	4.81435200	2.23035200	0.05314000
H	2.52519900	3.25028200	0.16665300
C	-0.22609700	-1.27210900	-2.19022800
O	-0.28221800	-1.55598300	-3.33303300
C	-1.76859600	-1.67784800	-0.10559500
C	0.55877600	-2.53918700	0.00201700
O	-2.81166200	-2.17073500	0.12233100
O	1.02578500	-3.57962400	0.29470700
O	-0.18346000	3.10170300	0.09059100
C	-1.58820200	3.13753300	-0.26941400
C	-2.07507600	1.66609400	-0.14892000
H	-2.09562000	3.82469900	0.40984700
H	-1.66619200	3.50949500	-1.29782900
C	-2.76587400	1.42420100	1.20587400
H	-3.69388600	2.00457600	1.26122900
H	-3.01084400	0.36750600	1.33307700
H	-2.11640000	1.72999700	2.03192700
C	-3.00133300	1.29745000	-1.31248500
H	-3.34781100	0.26512400	-1.22677000
H	-3.87981700	1.95284900	-1.31320900
H	-2.48407100	1.41114700	-2.26994200
C	-0.11486200	-0.86209500	2.57070900
O	0.46005900	0.17017300	2.68680600
O	-0.67206400	-1.85235600	2.92617600
C	-3.00133300	1.29745000	-1.31248500
H	-3.34781100	0.26512400	-1.22677000
H	-3.87981700	1.95284900	-1.31320900
H	-2.48407100	1.41114700	-2.26994200
C	-0.11486200	-0.86209500	2.57070900
O	0.46005900	0.17017300	2.68680600
O	-0.67206400	-1.85235600	2.92617600

#### 4

Mn	-0.13257700	-1.03278300	-0.27408300
N	-0.85608200	0.90688900	-0.17113500
N	1.64330500	0.06319000	-0.23465700
C	2.90586200	-0.39162500	-0.33266100
C	4.02018100	0.43693800	-0.22621600
C	3.83483400	1.80845200	-0.01566800
C	2.53534800	2.29808500	0.07208200
C	0.07381500	1.78139900	-0.00621600
C	1.47211300	1.39652400	-0.03723800
H	3.02354400	-1.45632900	-0.49786100

H	5.01285500	0.00803600	-0.30813600
H	4.68482800	2.47746000	0.07004000
H	2.33116900	3.35209300	0.22185200
C	-0.19130400	-1.15227500	-2.06601700
O	-0.24464100	-1.31398600	-3.22174500
C	-1.71772500	-1.81871000	-0.04382600
C	0.69535900	-2.59328500	-0.04343200
O	-2.74208900	-2.35581900	0.10998200
O	1.23016000	-3.61776100	0.12455400
O	-0.28401500	3.07358600	0.14969800
C	-1.72845300	3.10598200	-0.05369200
C	-2.16827800	1.60929600	-0.11093800
H	-2.16930700	3.65620700	0.77910200
H	-1.91537000	3.63838900	-0.99047800
C	-2.92989700	1.20925100	1.16346900
H	-3.85156800	1.79670600	1.23743700
H	-3.19793500	0.15109200	1.14510100
H	-2.32058800	1.39500900	2.05209500
C	-2.99689300	1.31400600	-1.36734900
H	-3.26348800	0.25513100	-1.41717300
H	-3.92297900	1.89885400	-1.34999300
H	-2.44001200	1.57580900	-2.27227000
C	-0.04992600	-0.93955000	1.95246900
O	0.39844800	0.13696800	2.42401700
O	-0.44505200	-1.93628400	2.62778200

## 5

Mn	-1.45738300	0.07275400	-1.09637400
N	-1.34702500	-1.21787300	0.53077500
N	-1.97413600	1.35121500	0.48234700
C	-2.34179200	2.64229600	0.41892100
C	-2.60024200	3.41171000	1.55221300
C	-2.48305500	2.82583200	2.81603800
C	-2.11445500	1.48533000	2.89775300
C	-1.51082000	-0.62006400	1.65716900
C	-1.86453400	0.78974000	1.71262600
H	-2.42860800	3.07266700	-0.57193100
H	-2.88902400	4.45054900	1.43664800
H	-2.68056600	3.40001800	3.71528000
H	-2.01803500	0.97664900	3.85001300
C	-3.17173200	-0.33422200	-1.49230100
O	-4.26146000	-0.58466800	-1.82227400
C	-0.78603400	-1.07982700	-2.28362300
C	-1.34978800	1.39302700	-2.29064400

O	-0.34183700	-1.81278800	-3.07298800
O	-1.25887600	2.25425200	-3.07154900
O	-1.39224300	-1.34267200	2.78852900
C	-1.21924900	-2.72539800	2.35247800
C	-1.01328600	-2.64366000	0.80737300
H	-0.35980300	-3.13620600	2.88424900
H	-2.12494600	-3.27080300	2.63120100
C	0.44903900	-2.92891800	0.42836200
H	0.70510900	-3.95668900	0.70763500
H	0.60541700	-2.81681100	-0.64640400
H	1.12432700	-2.24430300	0.94863300
C	-1.97268400	-3.57895800	0.06126900
H	-1.84073500	-3.49079700	-1.02017100
H	-1.77428800	-4.61831800	0.34452500
H	-3.01378700	-3.34671900	0.30552100
C	0.60099400	0.58590300	-0.63466900
O	0.90453600	0.76626800	0.57045200
O	1.45157200	0.69485800	-1.59832700
H	2.87693600	1.18472400	-1.24196000
C	5.11126400	0.10453000	0.38437000
C	4.17846500	1.30069200	0.25461100
F	6.27526500	0.26250500	-0.30303800
F	5.45620800	-0.10875200	1.68659900
F	4.55539400	-1.05136300	-0.06622500
O	3.82740500	1.53751000	-1.07913600
H	3.29549400	1.09298500	0.87408000
H	4.71807100	2.15912100	0.67485200

#### TS5\_6

Mn	1.73432800	-0.94569700	-0.92209000
N	2.92937100	0.59096600	-0.17574200
N	2.07726600	-1.60055100	1.04488500
C	1.67508100	-2.74608800	1.61897700
C	1.90406700	-3.03808800	2.96348500
C	2.58424300	-2.11081600	3.75618800
C	3.01798000	-0.92291600	3.17078700
C	3.17182500	0.47127900	1.08031500
C	2.74058500	-0.70762500	1.82009300
H	1.15153800	-3.44981900	0.98254400
H	1.55162200	-3.97879800	3.37182400
H	2.77697200	-2.31157400	4.80488100
H	3.55916200	-0.17236700	3.73511800
C	3.14050900	-1.87313300	-1.59335300
O	4.00412300	-2.48835900	-2.07192600



C	1.37014300	-0.15315400	-2.48344800
C	0.55409300	-2.23776800	-1.28134200
O	1.11324100	0.34989600	-3.50090100
O	-0.22799600	-3.06835900	-1.51384200
O	3.87494800	1.44155900	1.69213400
C	4.28379900	2.35773500	0.62988700
C	3.50493400	1.88605700	-0.63800100
H	4.02686700	3.36908000	0.94788900
H	5.36754900	2.26531100	0.52051400
C	2.37804600	2.86875100	-0.99510900
H	2.81073100	3.83967600	-1.25926700
H	1.79853500	2.50940800	-1.84813600
H	1.69925100	3.00511000	-0.14890200
C	4.44714100	1.66526000	-1.82745400
H	3.89616700	1.30695700	-2.70089700
H	4.93309300	2.60932100	-2.09601500
H	5.22335600	0.93462900	-1.58072400
C	0.09037900	0.13407900	-0.10373000
O	0.17425800	0.66618400	1.02249500
O	-1.01334200	0.22069800	-0.81494100
H	-1.96883900	0.80756900	-0.28923000
C	-2.83470200	3.70859600	0.45668000
C	-2.69702900	2.31449100	1.05421800
F	-4.08021500	3.95778100	-0.03232500
F	-2.58594000	4.67307400	1.39004400
F	-1.97056600	3.93108500	-0.56997300
O	-2.96052400	1.32343000	0.11128500
H	-1.67352000	2.23591900	1.44926200
H	-3.39950500	2.27508800	1.89984200
C	-4.94130700	-2.29137600	-0.17889100
C	-4.90126500	-1.26028000	0.94400400
F	-4.02367600	-2.04559000	-1.14900400
F	-4.68907800	-3.54190600	0.29762900
F	-6.15060300	-2.34319500	-0.79576000
O	-5.17801500	0.02719300	0.47054300
H	-4.31217100	0.51788700	0.30480100
H	-5.65694600	-1.56567200	1.67672600
H	-3.91246800	-1.33739200	1.41388800
<b>6</b>			
Mn	0.16605600	-1.02086300	0.26406400
N	0.82159700	0.96235500	0.12178900
N	-1.66424200	0.03307400	0.19320200
C	-2.90667900	-0.46839100	0.26450700

C	-4.04799900	0.32820000	0.15489400
C	-3.90391000	1.70257000	-0.03451100
C	-2.61720600	2.23707600	-0.10402700
C	-0.13832100	1.80414200	-0.01858900
C	-1.53262900	1.36962900	0.01200000
H	-2.99300500	-1.53829400	0.41170500
H	-5.02697000	-0.13342100	0.21843100
H	-4.77311400	2.34558700	-0.12291100
H	-2.44607600	3.29793200	-0.24405700
C	0.19114600	-0.96614600	2.09003200
O	0.21381100	-0.96824300	3.24760800
C	1.79619100	-1.77307700	0.17654400
C	-0.60109000	-2.64362700	0.22945700
O	2.83915800	-2.27763700	0.11542100
O	-1.09069400	-3.69548000	0.19375500
O	0.16336100	3.10175900	-0.16686500
C	1.61941100	3.18842800	-0.05287900
C	2.11113500	1.70946000	0.05953600
H	1.98783600	3.69988800	-0.94334000
H	1.83970000	3.78192800	0.83715100
C	2.90616900	1.29253400	-1.18715100
H	3.80882000	1.90744100	-1.26622900
H	3.21221600	0.24570200	-1.12842000
H	2.30975400	1.43008100	-2.09335200
C	2.92238700	1.48021500	1.34124600
H	3.21895400	0.43231000	1.43387400
H	3.83189300	2.08969200	1.31821500
H	2.34292600	1.75886100	2.22651100
C	0.08259800	-0.99429300	-1.81088400
O	-0.34386100	-0.08806700	-2.52270600
O	0.55512100	-2.12202200	-2.46145400
H	0.45177700	-1.96690800	-3.42121000

7

Mn	0.19625700	-1.01744600	0.28360600
N	0.78988600	0.99444900	0.14146600
N	-1.67771400	-0.05649900	0.11363300
C	-2.91002900	-0.58757000	0.13470200
C	-4.08439100	0.15029400	0.02269000
C	-3.98352400	1.56973500	-0.11758200
C	-2.73631700	2.15079300	-0.13520000
C	-0.24578300	1.79842000	-0.01808000
C	-1.57303600	1.33599000	-0.01755800
H	-2.96066700	-1.66779500	0.24350900

H	-5.04419300	-0.35407800	0.04220500
H	-4.87782700	2.18026300	-0.20546000
H	-2.61500800	3.22520000	-0.23508600
C	0.09596600	-0.85331700	2.09253100
O	0.03006900	-0.76530100	3.24850200
C	1.85629300	-1.68299400	0.33762300
C	-0.50655400	-2.65779400	0.27336600
O	2.92862500	-2.13571000	0.38079600
O	-0.95938900	-3.73198500	0.25000800
O	0.06105300	3.12823100	-0.18694200
C	1.47022100	3.24003300	0.12915400
C	2.02822100	1.79147000	0.03130100
H	1.92359300	3.93483500	-0.58097000
H	1.56220100	3.64136200	1.14565800
C	2.71654500	1.54724000	-1.32638000
H	3.62590400	2.15406200	-1.40992900
H	2.99421100	0.49460300	-1.43168100
H	2.04811700	1.80810400	-2.15279900
C	3.00256600	1.50775800	1.18374400
H	3.39830500	0.49079200	1.12301000
H	3.85115400	2.20065800	1.14265000
H	2.50529200	1.62957100	2.15123000
C	0.23284700	-1.09846600	-1.79590100
O	-0.31822400	-0.36332500	-2.61335500
O	0.98430500	-2.14174300	-2.34840800
H	0.90763700	-2.05795100	-3.31945000

## 8

Mn	0.62048400	-0.08764700	0.79928100
N	2.28483900	-0.90085500	-0.19420400
N	1.62442300	1.66983900	0.19251500
C	1.30582500	2.95361900	0.42288500
C	2.05109500	4.03873900	-0.02631000
C	3.23983900	3.78169700	-0.77821600
C	3.60299700	2.47790100	-1.02599200
C	3.05143100	0.04134100	-0.71328800
C	2.79390200	1.41168500	-0.53724700
H	0.39932400	3.12348300	0.99769200
H	1.72374000	5.04847000	0.19550400
H	3.84859200	4.60313400	-1.14535300
H	4.50007300	2.23864400	-1.58897200
C	1.57883400	-0.07727800	2.34783900
O	2.18120200	-0.06615800	3.33906800
C	-0.14140700	-1.66549900	1.16924100

C	-0.74891000	0.80831600	1.51199800
O	-0.64462800	-2.68449000	1.42122600
O	-1.64658200	1.39698600	1.96630800
O	4.12547800	-0.40888000	-1.44307800
C	4.20035200	-1.83132400	-1.17967300
C	2.80307100	-2.21797900	-0.61625600
H	4.45258100	-2.33676500	-2.11432500
H	4.99548200	-2.00185700	-0.44384300
C	1.90955500	-2.83248200	-1.71207600
H	2.30228400	-3.80713700	-2.02491200
H	0.89044400	-2.97547100	-1.34180900
H	1.86461500	-2.17896700	-2.58887500
C	2.94491900	-3.18730000	0.56608100
H	1.96682900	-3.46526900	0.96687900
H	3.44877600	-4.10647100	0.24500600
H	3.53372200	-2.73434500	1.37000300
C	-0.34526200	-0.03191700	-1.03646800
O	0.03931800	0.41970900	-2.10705800
O	-1.64984800	-0.60048300	-1.08880200
H	-1.96032100	-0.50209700	-2.01029200
C	-5.57923200	0.19581600	-0.53200500
C	-4.63118000	0.05082400	0.65323700
F	-6.43737600	-0.84927400	-0.64545800
F	-6.33517000	1.31943500	-0.41255400
F	-4.91870900	0.28502600	-1.71615700
O	-3.84392300	-1.10920800	0.55180700
H	-3.04267100	-0.91804000	0.01794800
H	-4.03227100	0.96657900	0.711179300
H	-5.24995700	-0.01904700	1.55260900

#### TS8\_9

Mn	0.56079400	0.08544200	0.45667500
N	2.23402100	-1.04393000	-0.09865000
N	1.95422100	1.61290900	0.04739400
C	1.79059800	2.94836500	0.10296000
C	2.79580800	3.86480700	-0.17119500
C	4.08836100	3.37469100	-0.53385100
C	4.29209300	2.01616600	-0.60025900
C	3.28711000	-0.27847900	-0.34188400
C	3.22002700	1.12550900	-0.30845500
H	0.80074600	3.29732300	0.38137800
H	2.58797100	4.92692200	-0.10692200
H	4.89687200	4.06515400	-0.75480900
H	5.25716300	1.60084900	-0.87294400

C	1.15188500	0.09415500	2.18578900
O	1.54966700	0.11974300	3.26877500
C	-0.52887300	-1.32873200	0.74170900
C	-0.78026700	1.23906400	0.83027400
O	-1.23344400	-2.22305700	0.95295100
O	-1.62643600	1.98398900	1.09323400
O	4.44866300	-0.94756300	-0.61724800
C	4.06714500	-2.33789600	-0.77572700
C	2.67136900	-2.45826400	-0.10211400
H	4.01993500	-2.55775100	-1.84843500
H	4.83594100	-2.95493500	-0.30688300
C	1.74302400	-3.35153500	-0.93562900
H	2.17422800	-4.35419400	-1.03519000
H	0.76391700	-3.45699400	-0.46198900
H	1.60163600	-2.93603300	-1.93794900
C	2.79082300	-2.99286500	1.33849400
H	1.81882300	-2.97327900	1.84024500
H	3.15066100	-4.02810600	1.33420000
H	3.49158400	-2.38646300	1.92196700
C	0.18782200	0.14254800	-1.50465500
O	0.53126500	0.22791100	-2.60411100
O	-2.00510000	0.06494100	-1.78052000
H	-2.00287800	0.15567700	-2.74421500
C	-5.78291600	0.18138500	0.04725100
C	-5.19451900	-0.20142200	-1.30658800
F	-4.89363100	0.82118200	0.85079900
F	-6.85125400	1.01839100	-0.09710200
F	-6.22858000	-0.89527500	0.74993700
O	-4.11832000	-1.07104400	-1.17469200
H	-3.19737000	-0.56935700	-1.42586500
H	-6.02058700	-0.65352500	-1.87547200
H	-4.92229300	0.74279700	-1.80175600

**9**

Mn	0.05655500	1.12841800	-0.00930400
C	0.03025400	0.97329500	1.85981500
O	-0.01300200	0.84026200	2.99753800
N	0.94746200	-0.76116700	-0.08911300
N	-1.64667100	-0.10692800	-0.00634100
C	-2.94855000	0.24320900	0.00582800
C	-3.99157000	-0.66951600	0.01231000
C	-3.68272000	-2.06469300	0.00338300
C	-2.36526400	-2.45698700	-0.01064000
C	0.04541100	-1.73299100	-0.03730400

C	-1.33517400	-1.47416600	-0.01441800
H	-3.15979000	1.30794700	0.01102900
H	-5.01565200	-0.31435300	0.02367500
H	-4.47796900	-2.80384000	0.00588900
H	-2.08562400	-3.50556100	-0.02032000
C	0.00788700	1.04432900	-1.88532400
O	-0.03582700	0.93967900	-3.02567300
C	1.61534200	2.06410100	0.00391800
C	-0.90637200	2.66797600	0.03227800
O	2.58944100	2.68379900	0.02008700
O	-1.51134200	3.65136500	0.05899400
O	0.55397500	-2.99894700	-0.00391200
C	1.97267000	-2.85818700	-0.27754400
C	2.29837800	-1.36323300	-0.00097500
H	2.14313900	-3.12384700	-1.32684100
H	2.51108500	-3.55133200	0.37103000
C	3.25106600	-0.81144700	-1.06946500
H	3.50145700	0.23492300	-0.87760900
H	4.18740300	-1.38058000	-1.06856700
H	2.80348200	-0.88647500	-2.06518700
C	2.88926200	-1.17235000	1.40911300
H	3.86967800	-1.65654700	1.48039700
H	3.02030200	-0.11003800	1.63593000
H	2.23338300	-1.60936000	2.16924300

## 10

Mn	0.64967100	-0.08538600	0.80599800
N	2.28126300	-0.89565200	-0.22936300
N	1.69965100	1.65671200	0.22544500
C	1.39275100	2.93329000	0.50127200
C	2.14452200	4.00841700	0.02346800
C	3.26316900	3.75782900	-0.77067800
C	3.59679200	2.43402000	-1.05857600
C	3.04325000	-0.00290600	-0.75165600
C	2.79006500	1.42112900	-0.54411700
H	0.52083600	3.10283400	1.12159000
H	1.84727800	5.01968800	0.27746800
H	3.86581500	4.57366600	-1.15541000
H	4.45833800	2.18093300	-1.66515900
C	1.55836200	-0.15945900	2.39198300
O	2.10414800	-0.20926000	3.41056400
C	-0.17078700	-1.65623300	1.11378200
C	-0.72088600	0.81507700	1.53751900
O	-0.70596500	-2.66474500	1.31600600

O	-1.61115800	1.39719900	2.00151900
O	4.09761700	-0.40382000	-1.47479500
C	4.11625600	-1.86335700	-1.37527200
C	2.80125000	-2.23881400	-0.62052600
H	4.16286800	-2.26112700	-2.38973900
H	5.01822800	-2.13817400	-0.82365400
C	1.80256300	-2.93937400	-1.55489400
H	2.22381300	-3.89302000	-1.89003200
H	0.86070700	-3.14616800	-1.04159100
H	1.59163200	-2.32338300	-2.43352800
C	3.09240000	-3.08735800	0.62351900
H	2.17198800	-3.32515900	1.16254400
H	3.56199900	-4.03033100	0.32451700
H	3.77126200	-2.56415800	1.30350000
C	-0.27927700	0.05426800	-1.04029800
O	0.22460200	0.39982200	-2.10112100
O	-1.64392500	-0.27183600	-1.10460500
H	-1.92682400	-0.15217600	-2.03260100
C	-5.65274800	0.17388200	-0.53323400
C	-4.71709500	0.01113300	0.65958300
F	-6.39594900	-0.93599300	-0.76756900
F	-6.52079900	1.19985400	-0.33151100
F	-4.98057900	0.44132500	-1.68397200
O	-3.83145800	-1.06678300	0.48306700
H	-3.05196900	-0.77490400	-0.03170200
H	-4.20094200	0.96647100	0.80759500
H	-5.34166400	-0.18830800	1.53481600

#### TS10\_11

Mn	0.77568700	-0.47499700	0.67486000
N	2.61765900	-0.49831800	-0.34945300
N	1.14407900	1.59065300	0.36965100
C	0.35783500	2.61328200	0.73306300
C	0.70633800	3.94498700	0.49058700
C	1.90452300	4.23087400	-0.15997900
C	2.72538400	3.17117900	-0.55246900
C	3.06716000	0.67650100	-0.62337800
C	2.30788900	1.87501400	-0.26602400
H	-0.57697600	2.36093700	1.21449600
H	0.03599500	4.73473500	0.81030200
H	2.19664900	5.25584500	-0.36187500
H	3.66465900	3.33505600	-1.06721500
C	1.68568100	-0.39092200	2.28290400
O	2.24837400	-0.33620800	3.28352400

C	0.59876300	-2.27561300	0.82066000
C	-0.82384100	-0.24038600	1.53386800
O	0.46693300	-3.41784500	0.92321000
O	-1.80141400	-0.13768500	2.13201500
O	4.24582900	0.78161700	-1.23829300
C	4.69737600	-0.59026100	-1.48515100
C	3.62864000	-1.50334100	-0.80253100
H	4.74540000	-0.72273200	-2.56767600
H	5.69305100	-0.68763700	-1.05070900
C	3.01099900	-2.48233400	-1.80887300
H	3.79212100	-3.14118300	-2.20178400
H	2.25041100	-3.10920800	-1.33759400
H	2.55589300	-1.94835100	-2.64762100
C	4.21121500	-2.24204500	0.41113700
H	3.44518700	-2.83440500	0.91799300
H	4.99987500	-2.92527600	0.07976700
H	4.64399500	-1.53967200	1.12976400
C	-0.08388500	-0.53348500	-1.09792100
O	-0.24456000	-0.82726400	-2.19726900
O	-1.88966300	0.91578200	-0.79568400
H	-1.66140400	1.58336700	-1.45761800
C	-5.81690800	-0.17535600	-0.21985000
C	-5.00213400	0.32962200	-1.40719800
F	-5.16142300	-0.05181500	0.96490500
F	-6.98764100	0.51503900	-0.08989800
F	-6.15515800	-1.48830200	-0.33434700
O	-3.82103900	-0.37974700	-1.56921200
H	-2.95666300	0.21781400	-1.22858500
H	-5.66270000	0.23560800	-2.28257900
H	-4.83773000	1.40389300	-1.22729300

## 11

Mn	0.07935900	1.10750800	0.00000500
C	0.05922600	1.05931600	1.88805200
O	0.03947100	1.02665000	3.03034400
N	0.90347000	-0.82055600	-0.00005300
N	-1.66103400	-0.10736900	0.00000300
C	-2.94129500	0.29347000	0.00003200
C	-4.00737000	-0.60934100	0.00004800
C	-3.74373100	-1.97702100	0.00003200
C	-2.41432300	-2.40487800	-0.00000400
C	0.01792200	-1.75650700	-0.00005400
C	-1.41098000	-1.44176100	-0.00001700
H	-3.12460800	1.36066400	0.00004400



H	-5.02236900	-0.22911800	0.00007400
H	-4.55296000	-2.69909900	0.00004600
H	-2.15208800	-3.45617700	-0.00002200
C	0.05924200	1.05934600	-1.88804700
O	0.03950000	1.02668400	-3.03033900
C	1.67507900	2.00471100	0.00003400
C	-0.83207800	2.69545800	0.00000700
O	2.66613400	2.58728500	0.00006300
O	-1.39305500	3.69908000	-0.00000200
O	0.42876100	-3.02120700	-0.00008300
C	1.89414900	-2.97544000	-0.00028800
C	2.25968200	-1.45489300	-0.00002000
H	2.23243300	-3.49978000	-0.89512900
H	2.23271000	-3.50017700	0.89421200
C	3.03067400	-1.06710700	-1.26896500
H	3.26100100	0.00099000	-1.28605400
H	3.97896500	-1.61295900	-1.29944300
H	2.46052800	-1.31927000	-2.16776500
C	3.03038300	-1.06746500	1.26921800
H	3.97874300	-1.61319700	1.29967600
H	3.26055100	0.00066000	1.28673300
H	2.46010300	-1.32003000	2.16782100

#### TS6\_12

Mn	0.56667200	0.49669500	-1.00705400
N	0.95702400	-0.89227600	0.51381000
N	-1.18257100	-0.69878200	-1.04562000
C	-2.24212100	-0.57443500	-1.85835900
C	-3.34722300	-1.42574200	-1.78861100
C	-3.35936400	-2.45078200	-0.84416300
C	-2.26069200	-2.59193800	0.00529800
C	0.00592100	-1.73831800	0.69297300
C	-1.20205200	-1.69790500	-0.12946300
H	-2.20911100	0.22743400	-2.58601400
H	-4.17661800	-1.27602900	-2.47052300
H	-4.20384100	-3.12742200	-0.76870800
H	-2.21551900	-3.37151100	0.75661200
C	1.35887300	-0.60819200	-2.25075500
O	1.85898300	-1.28033800	-3.04319600
C	2.08014200	1.45782800	-0.79870500
C	0.00145000	1.64102100	-2.28183400
O	3.03958900	2.09270100	-0.67628500
O	-0.35772100	2.38944100	-3.08850100
O	0.14627200	-2.66771000	1.64336300

C	1.46439300	-2.43998600	2.23871100
C	2.04677200	-1.19852900	1.48778300
H	1.31332000	-2.26695600	3.30546800
H	2.04995200	-3.34849700	2.08657200
C	2.25602000	-0.01542100	2.44360600
H	3.00388200	-0.28302600	3.19700500
H	2.61676700	0.86647700	1.90892600
H	1.32593300	0.24333200	2.95785600
C	3.34150800	-1.54996100	0.74194300
H	3.72069700	-0.69020700	0.18392700
H	4.10965700	-1.85035600	1.46189000
H	3.18036500	-2.37729300	0.04427800
C	-0.33686500	1.68230600	0.38200600
O	-1.18876200	1.10692300	1.26050900
O	-0.17271800	2.94681900	0.50053700
H	-0.83231900	3.25672900	1.36665400
C	-1.90334300	1.84424800	2.30431400
O	-2.62055300	1.15312700	3.00056800
O	-1.66654700	3.09805900	2.32633200

## 12

Mn	0.66232300	1.01577000	-0.40644300
N	0.89409300	-1.05799800	-0.19307300
N	-1.13983400	0.28455600	-1.24837300
C	-2.14219000	0.99610100	-1.78466600
C	-3.28570500	0.39935300	-2.32053400
C	-3.39951600	-0.98975100	-2.30648600
C	-2.36115300	-1.74124100	-1.75384900
C	-0.10539900	-1.73341300	-0.63666600
C	-1.25778900	-1.06590800	-1.23918800
H	-2.03074900	2.07369400	-1.78672800
H	-4.06532100	1.02569900	-2.73917300
H	-4.27592900	-1.47991000	-2.71672400
H	-2.39592200	-2.82366900	-1.71725300
C	1.45774200	0.96607100	-2.06296500
O	1.96399500	0.96127000	-3.10015700
C	2.21117100	1.47677900	0.39511400
C	0.22236500	2.75354300	-0.58940800
O	3.19500600	1.79441500	0.91538500
O	-0.05858700	3.87290700	-0.68526400
O	-0.06929300	-3.06707800	-0.54359300
C	1.21938300	-3.39345000	0.06900200
C	1.90396300	-2.01580500	0.34695200
H	1.01278500	-3.96325500	0.97644800

H	1.76936700	-4.01140300	-0.64321600
C	2.10529800	-1.78529800	1.85146200
H	2.78749700	-2.54362400	2.24928000
H	2.54226900	-0.80307700	2.04627700
H	1.15590100	-1.85868600	2.38959600
C	3.22644400	-1.88215500	-0.42045700
H	3.68048800	-0.90162400	-0.25678900
H	3.93210200	-2.64333200	-0.07186500
H	3.07208700	-2.02144900	-1.49460500
C	-0.23102300	1.07104500	1.44161200
O	-1.23987200	0.05160900	1.64456400
O	-0.03511800	1.83700100	2.38460000
H	-1.03976500	1.34381300	3.49526800
C	-1.98490700	-0.12768300	2.78523200
O	-2.80294200	-1.02364200	2.82654900
O	-1.76004100	0.70570700	3.79163700

**TS6\_13**

Mn	-0.33235000	0.13848500	0.66760100
N	1.18506400	-1.11560900	-0.07374000
N	1.15919900	1.53950400	0.09805100
C	1.11414600	2.87581000	0.20838900
C	2.15845900	3.70024700	-0.21674300
C	3.29632900	3.12430900	-0.77854100
C	3.35544300	1.73463000	-0.89680500
C	2.21203800	-0.47410200	-0.50672600
C	2.27051000	0.98629800	-0.44819600
H	0.22056700	3.30170200	0.64790800
H	2.06653700	4.77439600	-0.10303900
H	4.12198900	3.74076700	-1.11734800
H	4.21600700	1.23341700	-1.32375100
C	0.38929800	0.03409600	2.35224800
O	0.83282500	-0.02674400	3.41448800
C	-1.50325400	-1.19691900	1.03291400
C	-1.51071300	1.40629600	1.20824200
O	-2.21950600	-2.06719300	1.28290600
O	-2.22465400	2.23699200	1.57344500
O	3.23804000	-1.16861200	-1.00584900
C	2.86841700	-2.58015100	-0.88321200
C	1.43500300	-2.57756500	-0.25936500
H	2.90203300	-3.01259100	-1.88435700
H	3.61510000	-3.05520800	-0.24446700
C	0.40545800	-3.17714500	-1.22785200
H	0.65290100	-4.22664500	-1.41761800

H	-0.60265800	-3.13949600	-0.80862000
H	0.40741000	-2.64325100	-2.18244100
C	1.41474700	-3.29743200	1.09609200
H	0.42022800	-3.26409600	1.54751100
H	1.68557800	-4.34896600	0.95562100
H	2.13087800	-2.84725500	1.79003900
C	-0.95979100	0.27630600	-1.26131100
O	-0.48520200	0.28264300	-2.33797800
O	-2.69668300	0.54137100	-1.49667400
H	-2.79434500	0.57297700	-2.46391500
C	-4.32145400	0.18761900	-0.90587300
O	-4.28436800	0.10776400	0.29354000
O	-5.02184500	0.13766300	-1.89079000

### TS12\_13

Mn	-0.95895100	-0.84966700	0.36378300
N	-0.70814400	0.86995300	-0.80024700
N	0.79587000	-1.32257600	-0.72065600
C	1.52070300	-2.44857700	-0.66201100
C	2.67024800	-2.64284600	-1.43183000
C	3.08426200	-1.63660800	-2.30216300
C	2.33339200	-0.46149000	-2.37414400
C	0.33967800	0.82986400	-1.54323900
C	1.20515200	-0.34846600	-1.56820400
H	1.17791700	-3.21885300	0.01814100
H	3.21959300	-3.57297900	-1.34029800
H	3.97183200	-1.76057700	-2.91332600
H	2.60942400	0.35353300	-3.03269200
C	-1.96995300	-1.61176900	-0.97482700
O	-2.60771900	-2.09449800	-1.80201600
C	-2.45405900	-0.29218400	1.22527800
C	-0.96355400	-2.39500900	1.31155400
O	-3.40698600	0.04156500	1.78565000
O	-0.97156800	-3.37496200	1.92296800
O	0.62535000	1.89057400	-2.30200200
C	-0.43966800	2.86400400	-2.05428500
C	-1.37233700	2.19338600	-0.99385800
H	0.03415100	3.77881700	-1.69486900
H	-0.93665300	3.05010500	-3.00807600
C	-1.37885600	2.98423400	0.32208200
H	-1.77581500	3.98859500	0.14168000
H	-2.01261000	2.50290100	1.07091300
H	-0.36720300	3.07765700	0.72679600
C	-2.79413400	2.00338600	-1.53984500

H	-3.43291100	1.49604900	-0.81251200
H	-3.23892700	2.98090700	-1.75318600
H	-2.78480000	1.42016400	-2.46562000
C	0.12378000	-0.01779900	1.86500200
O	1.63426300	0.77179200	1.16947000
O	0.09891500	0.11988400	3.03418900
H	1.59342100	1.07104400	3.46560800
C	2.55061500	1.41992100	1.83164500
O	3.53880200	1.94533400	1.31640100
O	2.41027300	1.52561000	3.18562200

### 13

Mn	-0.08783500	0.06109400	0.67916900
C	-0.94002500	0.14183700	-1.01234200
O	-1.39739500	0.20797200	-2.05672400
N	1.46367100	-1.03355000	-0.21765500
N	1.21105000	1.60450000	0.02008300
C	1.04492300	2.92854400	0.15839700
C	1.97496800	3.85334300	-0.32254400
C	3.12032600	3.39593900	-0.97001300
C	3.30337600	2.01944700	-1.11885400
C	2.39912100	-0.29327900	-0.70325400
C	2.32918200	1.16552100	-0.61212600
H	0.14856600	3.26271500	0.66590900
H	1.78878900	4.91205500	-0.18341000
H	3.85799200	4.09274900	-1.35281200
H	4.17516200	1.60852300	-1.61391300
C	0.85414300	0.01266200	2.30571900
O	1.42853800	-0.00816800	3.29525600
C	-1.09325100	-1.38754300	1.17554100
C	-1.32788500	1.19612600	1.40168500
O	-1.71380800	-2.29570100	1.50838800
O	-2.09320700	1.91450000	1.87104700
O	3.43766000	-0.88292000	-1.29037600
C	3.18373600	-2.32498500	-1.21634800
C	1.82483900	-2.46626800	-0.45611100
H	4.02452500	-2.77344000	-0.68541200
H	3.14430800	-2.69713700	-2.24123700
C	2.00521200	-3.19611700	0.88184800
H	1.06474600	-3.24735900	1.43605700
H	2.34071000	-4.22127000	0.69553900
H	2.75373500	-2.69726600	1.50438700
C	0.76405100	-3.14835600	-1.33026800
H	1.08598000	-4.16824700	-1.56357100

H	-0.19696000	-3.21248400	-0.81414900
H	0.62298900	-2.60918100	-2.27145400
O	-3.98938000	-0.43258900	-0.11899200
C	-4.89193300	0.17218000	-0.73751600
O	-5.03749900	1.40194500	-0.96240000
O	-5.89901800	-0.66788300	-1.26173400
H	-6.52954500	-0.08522900	-1.71075100

**TS13\_14**

Mn	-0.17945500	-0.28806200	0.86451200
C	-0.89382500	0.24283900	-2.15094400
O	-1.33021400	0.23827300	-3.20289600
N	1.51834000	-0.71574300	-0.23812100
N	0.51091100	1.64815900	0.42516000
C	-0.03978000	2.81977700	0.77369400
C	0.51416200	4.04879600	0.40240300
C	1.68099900	4.06803900	-0.35681500
C	2.26494300	2.85205500	-0.72455500
C	2.15140200	0.33703400	-0.62790400
C	1.64951200	1.67608100	-0.31298800
H	-0.94584300	2.78006400	1.36538200
H	0.02567300	4.96575300	0.71138000
H	2.13222200	5.00691000	-0.65902800
H	3.17239800	2.80939000	-1.31513900
C	0.67918900	-0.36621900	2.42646000
O	1.25287400	-0.40176700	3.42826700
C	-0.76584200	-2.01388900	1.02500800
C	-1.71518000	0.27673300	1.69226300
O	-1.14910700	-3.09160700	1.15709300
O	-2.64990600	0.61611100	2.27262700
O	3.27661400	0.18559300	-1.32064500
C	3.48722200	-1.26009500	-1.44638900
C	2.29138900	-1.91675600	-0.68367100
H	4.45903000	-1.48315700	-1.00375200
H	3.49789700	-1.49128200	-2.51267700
C	2.77347000	-2.71557900	0.53523300
H	1.93065000	-3.13734500	1.08902000
H	3.40600600	-3.54472000	0.20215800
H	3.35849400	-2.08610600	1.21232500
C	1.44258500	-2.78461900	-1.62171700
H	2.04720500	-3.61731900	-1.99532100
H	0.57898900	-3.20363300	-1.10056300
H	1.08705100	-2.20605700	-2.47878900
O	-2.84542100	-0.86328900	-0.59747000

C	-3.83247100	-0.14153900	-0.88996000
O	-3.92399200	1.10689900	-0.95375300
O	-4.99539200	-0.86999900	-1.19254300
H	-5.67846900	-0.21549800	-1.40323400

**14**

Mn	0.14489600	-0.90826800	-0.49870400
N	-1.37345100	0.44538200	0.02521700
N	1.18588700	0.93805900	-0.53126300
C	2.47539300	1.14754000	-0.82846300
C	3.06725800	2.41170900	-0.75555900
C	2.29615900	3.50165300	-0.35756700
C	0.95041800	3.29466400	-0.04560700
C	-0.95250800	1.65372200	0.13646800
C	0.44137800	2.00295800	-0.14660800
H	3.05334500	0.28275100	-1.12950200
H	4.11551600	2.52362800	-1.00851800
H	2.72915200	4.49404000	-0.29127500
H	0.30536300	4.10698000	0.26777900
C	-0.29626200	-0.77493800	-2.24115600
O	-0.57408400	-0.67876600	-3.36059300
C	-0.83248400	-2.41760300	-0.28153700
C	1.59640500	-1.91834000	-0.93079400
O	-1.42962900	-3.39570700	-0.12940900
O	2.47130300	-2.57963200	-1.29442100
O	-1.82009100	2.60243500	0.50705600
C	-3.12000600	1.93665000	0.61166700
C	-2.82097700	0.41989600	0.38668500
H	-3.76424100	2.36533700	-0.15899300
H	-3.52197800	2.15815700	1.60113000
C	-3.65345000	-0.15188000	-0.76751200
H	-3.41495700	-1.20454600	-0.94005200
H	-4.71854300	-0.08254000	-0.52319600
H	-3.47535200	0.40400500	-1.69278500
C	-3.02349000	-0.38808300	1.67725100
H	-4.07904900	-0.35633100	1.96685700
H	-2.73979900	-1.43329800	1.53575500
H	-2.42529600	0.02456000	2.49438700
C	1.65231400	-1.06433200	2.10650100
O	2.74123000	-1.37170200	1.60781500
O	0.52152300	-0.86895200	1.53758700
O	1.61916800	-0.89771700	3.47997900
H	0.71015000	-0.66150800	3.72161200

## [Mn(benzox)(CO)<sub>3</sub>Br]

### Cat2

Mn	-0.81812500	-0.86372300	0.47153300
N	-1.51091200	1.13811800	0.29651100
C	-2.77881400	1.57124500	0.34551000
C	-3.12290900	2.91525100	0.18341400
C	-2.11630100	3.85427100	-0.03975500
C	-0.79167800	3.42026700	-0.09036400
C	-0.53688900	2.06016300	0.08111300
H	-3.54377000	0.82436700	0.52012800
H	-4.16585000	3.20668200	0.23351700
H	-2.35489800	4.90440900	-0.16927000
H	0.02798500	4.10927600	-0.25820100
C	-0.75249200	-0.75436400	2.26617700
O	-0.71314900	-0.68999200	3.42039100
C	-0.07346300	-2.51502500	0.45470200
C	-2.47524600	-1.59637000	0.48696600
O	0.38556700	-3.57503200	0.43005400
O	-3.52776500	-2.07308200	0.48255400
Br	-0.91423000	-0.99471300	-2.12643700
N	0.96914100	0.18518700	0.25404800
C	0.78400000	1.46692600	0.06809300
C	2.35099600	-0.00248700	0.18259800
C	3.16292500	-1.13520800	0.30647700
H	2.74671100	-2.11733900	0.49456500
C	4.53866800	-0.94298300	0.17631100
H	5.20197600	-1.79724000	0.26572400
C	5.09348400	0.33075800	-0.06763800
H	6.16999500	0.43080000	-0.16099000
C	4.29186900	1.46941700	-0.19200000
H	4.70465800	2.45413400	-0.37842600
C	2.92917200	1.25268600	-0.05971500
O	1.90995000	2.18342100	-0.12991500

### 1

Mn	-0.90302100	-1.08659100	-0.11138000
N	-1.72522000	0.83980400	-0.10437800
C	-3.03076900	1.17783500	-0.07344300
C	-3.47122600	2.49737900	-0.04409400
C	-2.53114700	3.53677500	-0.04290100
C	-1.17910000	3.21364400	-0.06482000
C	-0.81757400	1.86209800	-0.09374700



H	-3.73945800	0.35832100	-0.07252100
H	-4.53574000	2.70200600	-0.02468200
H	-2.84933400	4.57360300	-0.02254300
H	-0.40976000	3.97754800	-0.05815600
C	-1.14932900	-1.53487400	1.60539000
O	-1.32532000	-1.85811100	2.71282100
C	-0.03757800	-2.59993900	-0.53732000
C	-2.41811000	-1.84008800	-0.71189200
O	0.50508100	-3.59898800	-0.80211200
O	-3.40077700	-2.34385900	-1.09150500
N	0.78530100	0.07629300	-0.10233600
C	0.53123400	1.37012600	-0.09756600
C	2.18241600	-0.01720800	-0.06734600
C	3.05699700	-1.10790100	-0.04390500
H	2.69230500	-2.12788000	-0.05160000
C	4.42439300	-0.82546800	-0.01037300
H	5.13334100	-1.64712900	0.00864700
C	4.91002900	0.49751600	-0.00021000
H	5.98118100	0.67009100	0.02525200
C	4.04389000	1.59593600	-0.02115400
H	4.40265600	2.61885700	-0.01148000
C	2.69258500	1.28928500	-0.05257800
O	1.62595300	2.16795800	-0.07241300

## 2

Mn	-0.88521400	-1.07167600	-0.05451400
N	-1.72799800	0.76353900	-0.11649000
C	-3.06094700	1.08506700	-0.08897800
C	-3.54925700	2.37045300	-0.05750700
C	-2.64136900	3.47282400	-0.03954900
C	-1.29439000	3.20496300	-0.05125300
C	-0.84689700	1.85590500	-0.08851600
H	-3.74441500	0.24328400	-0.09515000
H	-4.62249600	2.53018200	-0.04586200
H	-3.00865400	4.49385000	-0.01252300
H	-0.55536000	4.00025700	-0.02926800
C	-0.94840700	-1.62113100	1.61036000
O	-1.01505300	-2.05261900	2.70446700
C	-0.00594700	-2.47116300	-0.71905600
C	-2.40075500	-1.85276000	-0.56711500
O	0.55432700	-3.41209200	-1.14896600
O	-3.39487000	-2.38350400	-0.90265700
N	0.74159600	0.10133000	-0.11341700
C	0.47428400	1.42140100	-0.09189400

C	2.13935200	0.02146200	-0.07249700
C	3.02215400	-1.06171700	-0.04876500
H	2.65908100	-2.08261300	-0.06330200
C	4.39553400	-0.78490800	-0.00842800
H	5.10070900	-1.61063500	0.00948300
C	4.88102400	0.53316600	0.01045900
H	5.95167700	0.71064200	0.04087500
C	4.00418500	1.62916100	-0.00709500
H	4.36230100	2.65302700	0.01202000
C	2.65173800	1.33122100	-0.04556400
O	1.60191100	2.22273500	-0.05930400

**3**

Mn	-0.79674500	-0.82993100	0.52438500
N	-1.51772500	1.12516800	0.28463900
C	-2.78523100	1.56994200	0.35699400
C	-3.15477100	2.89603000	0.16911300
C	-2.13956000	3.85192700	-0.11175900
C	-0.82886200	3.43783900	-0.18504200
C	-0.51961600	2.06237200	0.01475400
H	-3.54175800	0.82241900	0.57443000
H	-4.19893100	3.17944400	0.23677900
H	-2.39448900	4.89667000	-0.26281900
H	-0.02386400	4.13582000	-0.39138500
C	-0.69960200	-0.64277500	2.29144600
O	-0.63209900	-0.50451100	3.44190800
C	-0.04259000	-2.47068500	0.54627800
C	-2.44649900	-1.55989200	0.58776500
O	0.42110500	-3.53315200	0.55788300
O	-3.50157400	-2.03936100	0.62484400
Br	-0.96703100	-1.13157800	-2.16374600
N	0.97081300	0.18634500	0.22607600
C	0.75873800	1.49626100	-0.00302400
C	2.34188500	0.01103300	0.16761400
C	3.16926300	-1.10846400	0.33022100
H	2.75823000	-2.08664000	0.55109100
C	4.55343900	-0.92245000	0.19833000
H	5.21214700	-1.77753800	0.32069600
C	5.10963100	0.33431600	-0.08567800
H	6.18598200	0.43880100	-0.18004900
C	4.28951200	1.46710400	-0.24995700
H	4.69996000	2.44751700	-0.46775800
C	2.92957700	1.26195700	-0.11611500
O	1.92306200	2.20319000	-0.22465300

**Idimer**

Mn	-0.93942900	-0.01636900	-1.26457900
N	-1.78537300	1.84987600	-0.85643900
C	-1.29411300	3.06336800	-1.19010200
C	-1.98252500	4.24915200	-0.96391100
C	-3.25214100	4.20697500	-0.36740100
C	-3.78197900	2.97177900	-0.02031800
C	-3.02461000	1.82129800	-0.27735800
H	-0.31696900	3.07456800	-1.65713000
H	-1.52840800	5.18988100	-1.25476800
H	-3.80991300	5.11896700	-0.18328500
H	-4.75988700	2.87866100	0.43873000
C	-1.59274500	-0.05256200	-2.90677500
O	-1.96274200	-0.08165300	-4.01202100
C	-0.28986100	-1.68260600	-1.43333000
C	0.63905100	0.64400600	-1.79613400
O	0.11295300	-2.75837500	-1.62937200
O	1.63034800	1.05990400	-2.25356700
N	-2.67963300	-0.54740000	-0.30895500
C	-3.44314600	0.48109200	0.00229800
C	-3.42496800	-1.67399000	0.05994400
C	-3.17250600	-3.04641500	-0.03031500
H	-2.24801900	-3.42639600	-0.44661100
C	-4.16425400	-3.90928700	0.44170000
H	-4.00169300	-4.98114800	0.38738800
C	-5.37014100	-3.42673900	0.98799800
H	-6.11311500	-4.13334000	1.34393400
C	-5.63458000	-2.05583500	1.08042600
H	-6.55918400	-1.66962400	1.49441100
C	-4.63660200	-1.22026900	0.60316300
O	-4.63905700	0.15950300	0.56055700
Mn	0.93925300	-0.01551800	1.26417700
N	1.78641800	1.85007000	0.85546600
C	1.29583000	3.06395500	1.18866300
C	1.98517500	4.24922900	0.96261300
C	3.25507800	4.20606800	0.36680000
C	3.78423800	2.97044500	0.02018300
C	3.02591200	1.82053800	0.27695300
H	0.31847100	3.07591100	1.65521800
H	1.53155400	5.19032400	1.25306300
H	3.81359900	5.11763700	0.18286000
H	4.76232900	2.87657100	-0.43832100
C	1.59262200	-0.05166400	2.90634900

O	1.96269300	-0.08069200	4.01157300
C	0.28845600	-1.68118500	1.43336600
C	-0.63869700	0.64607400	1.79577100
O	-0.11501300	-2.75665000	1.62983200
O	-1.62978800	1.06259500	2.25308700
N	2.67920300	-0.54789700	0.30887700
C	3.44361200	0.47997300	-0.00224800
C	3.42391200	-1.67510800	-0.05940900
C	3.17030800	-3.04733000	0.03082900
H	2.24516000	-3.42648700	0.44640600
C	4.16165100	-3.91103100	-0.44050800
H	3.99822600	-4.98276000	-0.38618100
C	5.36822000	-3.42947900	-0.98617800
H	6.11086500	-4.13669700	-1.34157800
C	5.63374200	-2.05879100	-1.07870900
H	6.55884600	-1.67336700	-1.49231000
C	4.63615300	-1.22238600	-0.60210100
O	4.63957100	0.15739900	-0.55983800

**TS2\_4**

Mn	0.81047800	-0.96263100	-0.41582800
N	1.56606100	0.92219500	-0.33040700
C	2.86872600	1.31928700	-0.44624700
C	3.28051100	2.63421500	-0.40450600
C	2.31998400	3.66877300	-0.24239000
C	0.99245500	3.31465600	-0.14176200
C	0.63476600	1.94641300	-0.19149000
H	3.59382500	0.52342500	-0.57222900
H	4.33744600	2.86164100	-0.49563900
H	2.62493700	4.70960300	-0.20688300
H	0.21078300	4.05920400	-0.02871100
C	0.67153100	-1.39256800	-2.11645900
O	0.59722100	-1.75017700	-3.23408200
C	0.07057800	-2.43113200	0.26790900
C	2.41577900	-1.70462200	-0.20801900
O	-0.39753000	-3.41834300	0.70127700
O	3.46549000	-2.20790600	-0.06624700
N	-0.87676300	0.11817200	-0.20494900
C	-0.66947600	1.43314000	-0.11857000
C	-2.26474100	-0.03350000	-0.13298500
C	-3.09534600	-1.15660700	-0.18410000
H	-2.68629300	-2.15386400	-0.29715300
C	-4.47585800	-0.94686000	-0.08194000
H	-5.14469800	-1.80152700	-0.11791000

C	-5.01763000	0.34236900	0.06581500
H	-6.09350500	0.46523800	0.14270500
C	-4.19405300	1.47673900	0.11334600
H	-4.59721000	2.47772400	0.22285300
C	-2.83207400	1.24460100	0.00880900
O	-1.81793400	2.17887800	0.01815100
C	1.06312700	-0.53629300	2.50065800
O	0.37483200	0.42664500	2.62422000
O	1.78517200	-1.40783800	2.87764600

4

Mn	-0.85995600	-0.97030000	0.26208700
N	-1.60635500	0.98320900	0.24630200
C	-2.88850600	1.38485700	0.33645300
C	-3.27287100	2.71985700	0.25195000
C	-2.29338300	3.70528800	0.07130400
C	-0.96218100	3.31437600	-0.00958100
C	-0.66114800	1.94984300	0.07955200
H	-3.62826400	0.60536200	0.47710500
H	-4.32358500	2.97726000	0.32676800
H	-2.56587900	4.75325900	0.00295100
H	-0.16266800	4.03551200	-0.13738000
C	-0.91113400	-1.16464800	2.04805600
O	-0.97181700	-1.36627500	3.19616900
C	-0.05880000	-2.53702200	-0.03681100
C	-2.46481000	-1.70583400	-0.00095500
O	0.45175500	-3.56393500	-0.24872500
O	-3.50954000	-2.19019000	-0.18466600
N	0.88519500	0.11972300	0.21580600
C	0.66693200	1.40180400	0.04887700
C	2.27324200	-0.02252100	0.17737400
C	3.11430400	-1.13347100	0.30021000
H	2.71667900	-2.12930900	0.45571700
C	4.48958200	-0.90439100	0.21347300
H	5.17230300	-1.74345200	0.30440200
C	5.01583600	0.38711600	0.01060400
H	6.09137200	0.51942200	-0.05081000
C	4.18360600	1.50579400	-0.11196400
H	4.57485500	2.50517900	-0.26594100
C	2.82360600	1.25314300	-0.02217100
O	1.78528000	2.16022200	-0.09886700
C	-0.81579400	-0.78451800	-1.96836700
O	-0.39521200	0.32016200	-2.39642400
O	-1.20530000	-1.76052100	-2.67095800

## 5

Mn	0.73740400	0.64252100	1.19700300
N	1.34480400	2.05087300	-0.24042500
C	1.00080900	3.34761300	-0.32954200
C	1.41235300	4.17016800	-1.37631800
C	2.22453500	3.63933600	-2.38420500
C	2.60209500	2.30278600	-2.30299300
C	2.14024000	1.54633600	-1.22132300
H	0.37240600	3.73607000	0.46327500
H	1.09719000	5.20748300	-1.39415300
H	2.55945100	4.25717500	-3.21074800
H	3.23822000	1.84352300	-3.05115000
C	1.95122300	1.16181400	2.42978400
O	2.68315600	1.49018000	3.27448600
C	0.14994800	-0.74189900	2.16116400
C	-0.56115500	1.68299400	1.84814200
O	-0.25206400	-1.64079800	2.78319700
O	-1.41842200	2.35122000	2.26635200
N	2.07577100	-0.47015800	0.08459000
C	2.47852100	0.16546300	-0.98670800
C	2.63781200	-1.74405300	-0.01249100
C	2.58051600	-2.86972400	0.81602600
H	2.01416900	-2.86494000	1.73972200
C	3.28521000	-4.00160300	0.40050500
H	3.26388600	-4.89402600	1.01810100
C	4.02358400	-4.01818100	-0.80013200
H	4.55600700	-4.92030900	-1.08417300
C	4.08815100	-2.89773100	-1.63594000
H	4.65350900	-2.89575800	-2.56103000
C	3.38117600	-1.78707200	-1.20209400
O	3.27482300	-0.55473600	-1.81660400
C	-0.73535200	0.02084100	-0.28276500
O	-1.93311800	-0.24214200	0.10662600
O	-0.36060000	-0.05381400	-1.47806100
H	-2.98341500	-0.70535300	-0.93453500
C	-5.89437300	-0.67659400	-0.49386400
C	-4.72645100	-1.62994700	-0.72481700
F	-6.49805700	-0.29974900	-1.65199700
F	-6.85615600	-1.25897600	0.27641800
F	-5.52582200	0.46801300	0.13801400
O	-3.73934000	-1.05740300	-1.53090300
H	-4.35086100	-1.91608500	0.26645200
H	-5.14791500	-2.52275700	-1.20321400

**TS5\_6**

Mn	-2.26932800	-0.35999900	1.36281400
N	-2.28081600	-2.14901500	0.24420900
C	-2.02650100	-3.39544100	0.67550600
C	-1.99154200	-4.49824700	-0.17729100
C	-2.23378500	-4.31447300	-1.54137600
C	-2.50933300	-3.03079700	-2.00487500
C	-2.51977400	-1.98140500	-1.08261700
H	-1.84237900	-3.51245500	1.73691600
H	-1.77702900	-5.47979700	0.23020700
H	-2.21298700	-5.15468400	-2.22732500
H	-2.71286400	-2.83366400	-3.05121300
C	-3.95992900	-0.59385800	1.97948100
O	-5.02357900	-0.72403400	2.42981800
C	-2.09642800	1.26630900	2.08928400
C	-1.51627800	-1.11240100	2.80090600
O	-1.96317600	2.31937200	2.56444100
O	-1.01253000	-1.59441900	3.73180300
N	-2.88262000	0.32378300	-0.49567600
C	-2.82149900	-0.60833600	-1.41142100
C	-3.23803300	1.48739700	-1.17955800
C	-3.46104500	2.80284400	-0.75883000
H	-3.36423100	3.08990100	0.28138900
C	-3.81553800	3.73123700	-1.73958200
H	-3.99676600	4.76184900	-1.45112800
C	-3.94477100	3.36795900	-3.09573800
H	-4.22221100	4.12357300	-3.82372600
C	-3.72483600	2.05546600	-3.52724600
H	-3.82177700	1.76181300	-4.56631700
C	-3.37437600	1.15253100	-2.53551400
O	-3.10775800	-0.19624000	-2.67003700
C	-0.29058000	-0.09909900	0.61397800
O	0.63292700	0.34439000	1.44093200
O	-0.02229500	-0.36958000	-0.57306400
H	1.75428700	0.45719400	0.98636100
C	3.69194700	2.86865800	0.68643800
C	3.56777100	1.54052500	1.42616800
F	2.48478700	3.41344600	0.37727000
F	4.35571600	3.79354800	1.43835300
F	4.37397000	2.75931900	-0.48436800
O	2.91129100	0.58497700	0.65870800
H	4.59385500	1.23548600	1.67948300
H	3.04462500	1.76432200	2.36908000

C	6.03624000	-1.47369000	-1.11883700
C	4.54882100	-1.79415100	-1.01722700
F	6.80040100	-2.29868900	-0.35659100
F	6.47663400	-1.60339900	-2.40084500
F	6.32837200	-0.20620900	-0.72758100
O	4.08815400	-1.69669700	0.30043300
H	3.65673900	-0.79528000	0.44508400
H	4.02745900	-1.11373100	-1.70214700
H	4.42415900	-2.81840600	-1.38704000

**6**

Mn	0.87587600	-0.95014100	-0.24943300
N	1.58416000	1.04914700	-0.19463600
C	2.85672800	1.47120000	-0.24590300
C	3.20876200	2.81871500	-0.15341900
C	2.20528700	3.77683200	-0.00252200
C	0.87761400	3.35572400	0.04698100
C	0.61425600	1.98880500	-0.05105100
H	3.61797100	0.70916900	-0.36318400
H	4.25484800	3.09955000	-0.19988300
H	2.45041100	4.83091200	0.07169900
H	0.06015200	4.05887700	0.15743900
C	0.87840900	-0.96943900	-2.07784000
O	0.89470300	-1.01676200	-3.23391700
C	0.11351700	-2.57447400	-0.13974700
C	2.51347100	-1.68423300	-0.14852500
O	-0.36690600	-3.62653100	-0.05645900
O	3.56741200	-2.16199700	-0.07178200
N	-0.90708200	0.12401300	-0.17593600
C	-0.71137700	1.40943400	-0.03676900
C	-2.29235000	-0.04447000	-0.13594700
C	-3.11364500	-1.17308700	-0.23307500
H	-2.70215200	-2.16620900	-0.36668900
C	-4.49071300	-0.96194900	-0.15146100
H	-5.16084300	-1.81266700	-0.22280300
C	-5.03742400	0.32658400	0.02144100
H	-6.11494500	0.44185900	0.07948600
C	-4.22607400	1.46138700	0.11878800
H	-4.63297900	2.45742300	0.25034800
C	-2.86254100	1.22610200	0.03477600
O	-1.83542900	2.14852000	0.09427600
C	0.84295600	-0.83461500	1.82318100
O	1.27371200	-1.95388300	2.51119200
O	0.48218400	0.12570900	2.49974700



H	1.20443200	-1.75306100	3.46551700
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Mn	-0.87758600	-0.93778400	0.26609200
N	-1.59438200	1.05345300	0.11183100
C	-2.86114100	1.49392700	0.11794800
C	-3.22149500	2.83572000	0.02460700
C	-2.18772100	3.80687600	-0.08075500
C	-0.87434100	3.39484300	-0.08680600
C	-0.57681900	2.00338400	0.01096100
H	-3.63029800	0.73157700	0.20091400
H	-4.26858100	3.11640500	0.03319600
H	-2.43106800	4.86299100	-0.15405900
H	-0.05774600	4.10563400	-0.16389800
C	-0.83551000	-0.78321600	2.08159200
O	-0.82275500	-0.70922100	3.23929700
C	-0.11842100	-2.55903200	0.28332700
C	-2.51517600	-1.65721300	0.26618500
O	0.36102100	-3.61920800	0.28975300
O	-3.57840600	-2.13057900	0.25848300
N	0.92021200	0.11516300	0.11493500
C	0.70153000	1.43959800	0.01372300
C	2.28843700	-0.04767800	0.07894200
C	3.11842100	-1.17739500	0.14532500
H	2.70492800	-2.17441500	0.24496900
C	4.50558700	-0.97469400	0.07927900
H	5.16483000	-1.83694600	0.12924700
C	5.06429300	0.30582300	-0.04928300
H	6.14254700	0.42230200	-0.09706300
C	4.24176100	1.44918600	-0.11683300
H	4.65390800	2.44808400	-0.21567500
C	2.87985600	1.22900500	-0.05032200
O	1.87106900	2.17252000	-0.09221200
C	-0.89625300	-1.00194100	-1.80965900
O	-1.33304300	-2.19906000	-2.37812900
O	-0.57388400	-0.12325200	-2.60702200
H	-1.28973600	-2.08410100	-3.34802700

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Mn	-0.47405800	-0.73148900	0.76330700
N	-2.01835700	-1.84130900	-0.17916500
C	-2.12707400	-3.16985800	-0.33122500
C	-3.19806300	-3.79809200	-0.96055800
C	-4.24939700	-2.98908000	-1.47351600

C	-4.17615900	-1.62163600	-1.33446600
C	-3.04812600	-1.04367900	-0.68091000
H	-1.31231500	-3.76442900	0.07117800
H	-3.21519500	-4.87843500	-1.04839500
H	-5.10193600	-3.44465800	-1.96897800
H	-4.95888000	-0.97120100	-1.71153800
C	-1.37144700	-0.84708800	2.34799100
O	-1.92378700	-0.92741400	3.36361000
C	0.77736200	0.35662300	1.43787300
C	0.51069100	-2.18527600	1.11591000
O	1.59698800	1.05830700	1.87310400
O	1.14742400	-3.13178000	1.34242800
N	-1.74474700	0.80783500	0.14950800
C	-2.83294600	0.32159300	-0.47672400
C	-1.88651800	2.17956900	0.14738600
C	-1.09121100	3.22362100	0.64358200
H	-0.15444200	3.02550800	1.15148200
C	-1.54903300	4.53774700	0.46152100
H	-0.94720800	5.35996200	0.83870700
C	-2.75785800	4.81982300	-0.19237900
H	-3.07828100	5.84980200	-0.31453600
C	-3.56656100	3.78013700	-0.69513100
H	-4.50468600	3.97674200	-1.20373000
C	-3.09878200	2.49436900	-0.50618600
O	-3.69864600	1.31378500	-0.90141300
C	0.41768500	-0.58938800	-1.10108600
O	1.82753800	-0.72872600	-1.14871500
O	-0.10440500	-0.40042900	-2.19243100
H	2.08975200	-0.63994400	-2.08599600
C	5.63707200	0.46867800	-0.60808400
C	4.76461700	0.12524000	0.59416000
F	4.91798900	0.57429900	-1.75621600
F	6.26936700	1.65786600	-0.42360400
F	6.59911100	-0.46008000	-0.83798000
O	4.10453600	-1.10466000	0.42557500
H	3.27627300	-0.96714500	-0.08108900
H	5.42660200	0.05368200	1.46189400
H	4.07258600	0.96041300	0.74992300

#### TS8\_9

Mn	-0.58922800	-0.67192400	0.68079700
N	-2.11368500	-1.88107600	-0.15465800
C	-2.15389300	-3.22104300	-0.26586400
C	-3.21812400	-3.91924300	-0.82184100

C	-4.33714000	-3.18356000	-1.30256400
C	-4.33298300	-1.81115600	-1.20659900
C	-3.20871200	-1.15394000	-0.62809800
H	-1.28896800	-3.75823400	0.11004400
H	-3.18114500	-5.00091300	-0.87961500
H	-5.18598800	-3.69956000	-1.74110800
H	-5.16692900	-1.21477800	-1.56201400
C	-1.44949900	-0.77900500	2.29996600
O	-2.01316000	-0.84583300	3.30248000
C	0.63937400	0.50014000	1.31475700
C	0.49502200	-2.06945600	1.07575200
O	1.41822800	1.24124900	1.73912600
O	1.17817200	-2.96161400	1.34686600
N	-1.96111800	0.78033100	0.08686400
C	-3.05858500	0.22664300	-0.46879300
C	-2.17271900	2.14702600	0.06717600
C	-1.40572200	3.23898100	0.49528000
H	-0.43165800	3.10211300	0.95003400
C	-1.94232700	4.52264800	0.31571800
H	-1.36448900	5.38311400	0.64070900
C	-3.20061700	4.72590900	-0.27101800
H	-3.58181100	5.73488200	-0.39308700
C	-3.98006100	3.63681100	-0.70624300
H	-4.95493900	3.77286200	-1.16238300
C	-3.43369300	2.38156200	-0.52057000
O	-3.99301800	1.16245000	-0.85868900
C	0.09366500	-0.54228900	-1.17363400
O	2.35674600	-0.71235700	-1.01254500
O	-0.00850500	-0.43068000	-2.31545300
H	2.59741700	-0.65829600	-1.94809500
C	6.21083300	0.46794800	-0.48578300
C	5.00567900	0.38894200	0.44742800
F	5.88011000	0.29064100	-1.79329000
F	6.82608000	1.68343900	-0.40191800
F	7.16030200	-0.46438800	-0.20233000
O	4.37212100	-0.84391200	0.38148000
H	3.48443100	-0.78048700	-0.25980200
H	5.39424300	0.59363000	1.45599500
H	4.34806000	1.22582000	0.16527100

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Mn	0.87229800	-1.06824400	0.00001400
N	1.70208900	0.87418400	-0.00008500
C	3.00049500	1.23201600	-0.00014600

C	3.43479700	2.54967300	-0.0002110
C	2.46207300	3.58856200	-0.0002130
C	1.12631200	3.26151700	-0.0001470
C	0.74199100	1.88965100	-0.0000800
H	3.72240000	0.42198900	-0.0001450
H	4.49684400	2.76531900	-0.0002600
H	2.77131200	4.62929200	-0.0002630
H	0.35455900	4.02409100	-0.0001430
C	0.84340900	-0.96511100	-1.8775850
O	0.81403500	-0.86398200	-3.0178590
C	0.00507500	-2.67006500	0.0001090
C	2.49193300	-1.89916000	-0.0000590
O	-0.52755100	-3.69280900	0.0001590
O	3.51377800	-2.43393200	-0.0001090
N	-0.85660900	0.08643900	0.0000860
C	-0.56851800	1.40564500	0.0000000
C	-2.23821100	-0.00433400	0.0000950
C	-3.12674700	-1.08705700	0.0001720
H	-2.77288900	-2.11128700	0.0002260
C	-4.50022000	-0.80213600	0.0001770
H	-5.20688900	-1.62689800	0.0002330
C	-4.98501900	0.51446700	0.0001120
H	-6.05533900	0.69452400	0.0001190
C	-4.10177300	1.61038000	0.0000390
H	-4.45622300	2.63560100	-0.0000090
C	-2.75382800	1.30820100	0.0000320
O	-1.69366300	2.19769000	-0.0000270
C	0.84363400	-0.96499000	1.8776180
O	0.81440100	-0.86377500	3.0178870

## 10

Mn	-0.41830900	-0.64103200	0.62784500
N	-2.02939000	-1.89596500	0.03793400
C	-2.06059400	-3.23688600	0.01499100
C	-3.16911100	-3.95811300	-0.43236100
C	-4.29804200	-3.26775700	-0.87512800
C	-4.28391700	-1.87405800	-0.85242100
C	-3.13407400	-1.23278800	-0.39102600
H	-1.17307000	-3.75092800	0.36389400
H	-3.13524000	-5.04162600	-0.42886900
H	-5.17333400	-3.80239100	-1.22817600
H	-5.13592400	-1.28964600	-1.18006100
C	-0.93510300	-0.72479800	2.38314300
O	-1.22851200	-0.78043500	3.49980200

C	0.86409300	0.56786800	0.97997900
C	0.74683000	-1.99850100	0.82129900
O	1.69619200	1.34444000	1.20139400
O	1.49632400	-2.87457500	0.93880200
N	-1.89971100	0.75713500	0.18181400
C	-2.98469500	0.20322200	-0.29368500
C	-2.13606300	2.13249900	0.13390300
C	-1.36435100	3.24127300	0.49844300
H	-0.36878000	3.13160000	0.91079900
C	-1.93633600	4.49965400	0.30676700
H	-1.36909200	5.38448700	0.57730800
C	-3.23156400	4.65564000	-0.22924000
H	-3.63435600	5.65480900	-0.36004900
C	-4.01136800	3.55472500	-0.59670400
H	-5.00818200	3.65960800	-1.00937500
C	-3.42166800	2.31612700	-0.39726400
O	-3.95328200	1.06889900	-0.66452500
C	0.05071600	-0.54248500	-1.38673900
O	1.40672900	-0.58168800	-1.74040600
O	-0.73352100	-0.45295800	-2.32279600
H	1.45410400	-0.53042900	-2.71552900
C	6.03985500	0.43718500	-0.27377400
C	4.58941900	0.55951200	-0.70130300
F	6.76719500	-0.34898000	-1.10649200
F	6.63307000	1.65927400	-0.26092300
F	6.17545800	-0.08375800	0.97138700
O	4.01650200	-0.72867900	-0.68196000
H	3.09146000	-0.66780200	-0.99319200
H	4.10033400	1.24737600	-0.00062900
H	4.58438300	1.00977600	-1.70202900

#### TS10\_11

Mn	0.61632600	0.20498100	0.98800400
N	1.19657600	2.01543300	0.02048700
C	0.58571900	3.20760700	0.09002000
C	1.06162900	4.33558900	-0.58221300
C	2.21416100	4.23100400	-1.35953300
C	2.85985000	2.99717000	-1.44342900
C	2.31920200	1.92154400	-0.74131500
H	-0.30782700	3.26547000	0.69927700
H	0.52653400	5.27350800	-0.48868200
H	2.60493200	5.09130400	-1.89191900
H	3.75773100	2.86241200	-2.03516600
C	1.67071200	0.64667100	2.44801100

O	2.32272900	0.91840500	3.35345300
C	0.22530200	-1.43030100	1.69925300
C	-0.86628000	0.91229300	1.78691400
O	-0.00708400	-2.45716000	2.16506400
O	-1.78307200	1.36875000	2.31206500
N	2.32879100	-0.39262000	-0.05768200
C	2.87796500	0.58497100	-0.73544000
C	3.13586300	-1.50824300	-0.29480000
C	3.07501300	-2.83531600	0.14372500
H	2.28847400	-3.18430400	0.80133600
C	4.07825000	-3.69324100	-0.30690100
H	4.06726700	-4.73088900	0.01049000
C	5.10828500	-3.25158300	-1.16381100
H	5.86679400	-3.95694100	-1.48721100
C	5.17812700	-1.92815600	-1.60793100
H	5.96342100	-1.57498400	-2.26610300
C	4.17073800	-1.09523300	-1.14700500
O	3.98829200	0.24846100	-1.41799700
C	-0.38092600	-0.22146100	-0.64905000
O	-2.39671400	-1.07726300	0.25180400
O	-0.60650900	-0.32931800	-1.76923300
H	-2.45455800	-1.93835100	-0.18519900
C	-6.34385100	-0.64319300	-0.70864200
C	-5.34568900	0.18983500	0.09208300
F	-5.88293400	-1.89141000	-0.99426200
F	-7.51635600	-0.80970100	-0.02840400
F	-6.66955300	-0.07566300	-1.90190800
O	-4.15463700	0.37885100	-0.58800100
H	-3.34971100	-0.32883200	-0.20789600
H	-5.85828800	1.14134000	0.30402200
H	-5.21936400	-0.33852000	1.05164400

## 11

Mn	0.88965300	-1.04060600	0.00000700
N	1.66917600	0.94012400	-0.00009500
C	2.95918300	1.30914600	-0.00014700
C	3.35495100	2.64839000	-0.00020900
C	2.38332300	3.64774500	-0.00021800
C	1.03776600	3.27918400	-0.00016400
C	0.72669600	1.92110900	-0.00010400
H	3.69818600	0.51759000	-0.00013900
H	4.41197800	2.88790000	-0.00024900
H	2.66426000	4.69524700	-0.00026500
H	0.24388000	4.01692000	-0.00016800

C	0.87415600	-1.00066000	-1.89010000
O	0.86309800	-0.97678100	-3.03226700
C	0.05537300	-2.67243400	0.00010100
C	2.53397900	-1.84890800	-0.00001400
O	-0.45505100	-3.70172500	0.00016000
O	3.56081600	-2.36449500	-0.00002600
N	-0.85999700	0.10218000	0.00002100
C	-0.62118700	1.39134600	-0.00004000
C	-2.25284800	-0.01975200	0.00007700
C	-3.11336400	-1.12288600	0.00015500
H	-2.74232600	-2.14027800	0.00018400
C	-4.48158600	-0.85268900	0.00019500
H	-5.18238300	-1.68110100	0.00025600
C	-4.98229700	0.46629600	0.00016000
H	-6.05561000	0.62504800	0.00019400
C	-4.13184300	1.57503200	0.00008200
H	-4.50136000	2.59382000	0.00005400
C	-2.77752700	1.28120900	0.00004300
O	-1.71672200	2.16881100	-0.00003200
C	0.87427900	-1.00050900	1.89011300
O	0.86329600	-0.97653900	3.03227800

**[Mn(qinox)(CO)<sub>3</sub>Br]**

**Cat3**

Mn	0.90785700	-0.79967600	0.42351800
N	1.63140300	1.10776100	0.53136200
C	0.78441200	2.03705800	0.27393900
C	0.26776800	-2.46205200	0.06339900
O	-0.04658100	-3.54482000	-0.19454400
C	0.67647900	-0.94495300	2.20058000
C	2.56757300	-1.50369100	0.49498100
O	0.52866300	-1.03658300	3.34449500
O	3.63702200	-1.93959700	0.53486000
O	1.23400400	3.29358900	0.18193700
C	2.67112100	3.23538300	0.49633700
C	2.96591900	1.72108600	0.62460800
H	2.81838900	3.78714800	1.42599200
H	3.20211700	3.72325800	-0.32046900
H	3.59483800	1.34351300	-0.18734900
H	3.43629200	1.46307200	1.57658100
C	-0.63366400	1.72740900	0.09326800
C	-2.25300600	0.06793000	0.17929700
C	-3.27233400	1.03364100	-0.13645300

C	-2.89333900	2.38212400	-0.33283400
C	-1.57260400	2.73840500	-0.19549000
H	-1.91234800	-1.99385700	0.73951800
C	-2.65519100	-1.26700100	0.44872500
C	-4.63024000	0.62086500	-0.21582500
H	-3.64981700	3.12346800	-0.57137300
H	-1.23606800	3.76175600	-0.30846800
C	-4.98151900	-0.68727600	0.02999200
C	-3.98259200	-1.63141900	0.37787100
H	-5.38333200	1.36285700	-0.46401300
H	-6.02015000	-0.99677000	-0.02801200
H	-4.26660300	-2.65617700	0.59634400
N	-0.92908100	0.42990100	0.24622500
Br	1.16075500	-0.57930800	-2.16680400

**I**

Mn	1.06255400	-0.92815600	-0.04238600
N	1.97710100	0.84521000	0.01267800
C	1.18977400	1.88234400	-0.01223300
C	0.38167600	-2.04569700	-1.27261800
O	-0.01632900	-2.77985800	-2.08886400
C	0.59188200	-1.83742500	1.42654300
C	2.62147700	-1.80538700	-0.13307400
O	0.30698500	-2.43969600	2.38552700
O	3.63588200	-2.37642500	-0.18582800
O	1.75645300	3.09826300	-0.00326900
C	3.20869400	2.88031000	-0.02540100
C	3.36520400	1.34402700	0.07627800
H	3.63243500	3.42437900	0.81890500
H	3.58294800	3.29385700	-0.96342500
H	3.95351200	0.93082700	-0.74606300
H	3.82353900	1.03161900	1.01878100
C	-0.24116600	1.69807700	-0.03554600
C	-1.96049300	0.11935600	0.00085100
C	-2.93612200	1.17328700	-0.03605000
C	-2.48976800	2.52239700	-0.07488900
C	-1.14402300	2.78543500	-0.06495600
H	-1.70200800	-2.02239200	0.11943700
C	-2.42394800	-1.21953300	0.07016700
C	-4.31802300	0.84954000	-0.02459000
H	-3.21819400	3.32688200	-0.10438300
H	-0.75397100	3.79636800	-0.08204900
C	-4.73637400	-0.46369400	0.03196900
C	-3.77612700	-1.50144400	0.08494400



H	-5.03974100	1.66091500	-0.05741500
H	-5.79516200	-0.70276300	0.04141000
H	-4.10433400	-2.53501500	0.14040100
N	-0.60606900	0.39641500	-0.02051100

**2**

Mn	1.03066600	-0.92752600	-0.00135900
N	1.96147900	0.78226700	0.02640200
C	1.19801200	1.87586400	0.04432200
C	0.43288800	-1.90405000	-1.35051700
O	0.06625200	-2.57534400	-2.24498700
C	0.45577500	-1.91280300	1.34869900
C	2.59071300	-1.78841100	-0.01965300
O	0.10013500	-2.59126500	2.24230800
O	3.62298200	-2.34580100	-0.03175600
O	1.87306200	3.07524500	0.09283700
C	3.25488500	2.74378200	-0.21223900
C	3.36012200	1.24535500	0.12099500
H	3.89876800	3.38464800	0.39151700
H	3.42941100	2.93993000	-1.27661600
H	4.00651200	0.70952700	-0.57739200
H	3.73898200	1.07903400	1.13696300
C	-0.18476100	1.72360400	0.02670200
C	-1.93989600	0.12997700	0.00246100
C	-2.90866600	1.19058200	-0.00369600
C	-2.45059600	2.55701300	0.00182000
C	-1.11177200	2.80702600	0.01863400
H	-1.72220300	-2.01265300	0.00919400
C	-2.43237700	-1.19718300	0.00148000
C	-4.28602700	0.88240200	-0.01330000
H	-3.17905100	3.36286200	-0.00646500
H	-0.72062400	3.81986500	0.02502000
C	-4.73930600	-0.43154500	-0.01622700
C	-3.79531200	-1.47284100	-0.00794200
H	-4.99654500	1.70619500	-0.01825800
H	-5.80339700	-0.64883300	-0.02370500
H	-4.12741200	-2.50778200	-0.00816300
N	-0.56899900	0.38345100	0.01151600

**3**

Mn	0.85501700	-0.79467900	0.46381200
N	1.64981300	1.07120000	0.59194800
C	0.80614300	2.02914900	0.30583600
C	0.17187800	-2.41718300	0.04439900

O	-0.16901800	-3.48794400	-0.24616400
C	0.55316400	-0.95044900	2.20823700
C	2.48822300	-1.54273400	0.57056700
O	0.34629100	-1.03074500	3.34834600
O	3.54722800	-2.00962800	0.64543900
O	1.32383100	3.28865100	0.27423200
C	2.76910800	3.13509200	0.41566500
C	2.95486700	1.67217600	0.87573100
H	3.11470800	3.87668800	1.13678700
H	3.22213600	3.32865400	-0.56109300
H	3.75436000	1.16998700	0.32299400
H	3.18728700	1.59963600	1.94647600
C	-0.56434900	1.75611200	0.06882800
C	-2.24263900	0.09707000	0.17143200
C	-3.23970100	1.07077100	-0.20261000
C	-2.82056300	2.42482200	-0.45090500
C	-1.50130200	2.75613200	-0.28122200
H	-1.98733400	-1.93727200	0.84762300
C	-2.70041100	-1.20392800	0.49899500
C	-4.59307800	0.68717600	-0.28757800
H	-3.55840100	3.16927500	-0.73537100
H	-1.14996400	3.77435300	-0.41552500
C	-5.00555600	-0.61152800	0.00479200
C	-4.04617400	-1.55104400	0.41344800
H	-5.32268000	1.43885500	-0.58080800
H	-6.05384900	-0.88620800	-0.06600900
H	-4.35030700	-2.56117800	0.67510600
N	-0.90286300	0.41882700	0.22848000
Br	1.25644700	-0.62081400	-2.23477100

**Idimer**

Mn	-0.97955600	-0.28930100	-1.29885900
N	-1.83611200	-2.05299600	-0.82735700
C	-2.94146400	-1.99404200	-0.15725600
C	-0.07532500	1.25990900	-1.46055500
O	0.54856100	2.21861200	-1.69121200
C	-1.68379000	-0.14770700	-2.91222900
C	0.49394500	-1.11323200	-1.88928900
O	-2.09869700	-0.04601900	-3.99739000
O	1.42229100	-1.65690300	-2.33930400
O	-3.57657400	-3.15481500	0.10779200
C	-2.68983100	-4.21470900	-0.38029700
C	-1.62348400	-3.46086800	-1.20531200
H	-3.29410300	-4.90928600	-0.96340100

H	-2.27476300	-4.72281900	0.49338000
H	-0.60751000	-3.78229200	-0.97051000
H	-1.77182200	-3.56995100	-2.28503000
C	-3.48674100	-0.71348200	0.21259100
C	-3.31955500	1.59381100	-0.06710500
C	-4.50531700	1.78171600	0.72318600
C	-5.16309500	0.64190400	1.26112000
C	-4.67099100	-0.60438300	0.97770900
H	-1.88290000	2.61672700	-1.31135800
C	-2.74360100	2.73773900	-0.67353300
C	-5.01916600	3.08970700	0.92057100
H	-6.05745900	0.77110600	1.86304300
H	-5.15395600	-1.50870500	1.32917700
C	-4.41837200	4.18430000	0.33331000
C	-3.27985900	3.99681000	-0.48294800
H	-5.90933500	3.20759200	1.53228500
H	-4.82358300	5.18026200	0.48293600
H	-2.81905200	4.85102300	-0.97005700
N	-2.77332900	0.33474300	-0.26553500
Mn	0.97969600	-0.28960500	1.29918000
N	1.83674200	-2.05306300	0.82758600
C	2.94195100	-1.99379300	0.15726400
C	0.07523400	1.25957800	1.45989300
O	-0.54869700	2.21839200	1.68995900
C	1.68373200	-0.14733700	2.91259600
C	-0.49357500	-1.11369000	1.88991300
O	2.09849200	-0.04492500	3.99773900
O	-1.42192600	-1.65741800	2.33985500
O	3.57725900	-3.15444700	-0.10801800
C	2.69023800	-4.21450800	0.37921400
C	1.62471800	-3.46105900	1.20554300
H	3.29440300	-4.91015100	0.96114100
H	2.27445200	-4.72125200	-0.49491900
H	0.60853600	-3.78263800	0.97187700
H	1.77436700	-3.57024100	2.28508100
C	3.48691600	-0.71311300	-0.21259600
C	3.31935500	1.59408800	0.06744700
C	4.50461800	1.78238500	-0.72350700
C	5.16243100	0.64277500	-1.26179600
C	4.67081900	-0.60366800	-0.97818800
H	1.88332200	2.61642400	1.31289700
C	2.74347300	2.73780200	0.67439000
C	5.01794900	3.09055500	-0.92111600
H	6.05647400	0.77221000	-1.86414900

H	5.15389100	-1.50782700	-1.32992800
C	4.41718100	4.18491600	-0.33341700
C	3.27925400	3.99702800	0.48358900
H	5.90772600	3.20876300	-1.53334000
H	4.82198900	5.18101500	-0.48322100
H	2.81857000	4.85107500	0.97110300
N	2.77350800	0.33491800	0.26594000

**TS2\_4**

Mn	-0.84938300	-0.88483300	-0.36023300
N	-1.70791400	0.88644900	-0.50295100
C	-0.91409000	1.92271600	-0.34821700
C	-0.24113900	-2.16592000	0.71778100
O	0.10695900	-3.04320500	1.41830600
C	-0.36745500	-1.57017400	-1.91243200
C	-2.43734700	-1.69026900	-0.40580800
O	-0.05908200	-2.07903400	-2.92558600
O	-3.48428700	-2.21157700	-0.43999300
O	-1.50762700	3.15543400	-0.36467800
C	-2.86474500	2.92286600	-0.84226600
C	-3.07993900	1.40781600	-0.65083600
H	-2.90656100	3.21807500	-1.89582600
H	-3.53985700	3.54751500	-0.25655100
H	-3.66143500	1.18187200	0.24974100
H	-3.58317500	0.94997600	-1.50563400
C	0.46548600	1.70524400	-0.15672700
C	2.15670600	0.07135600	-0.08288700
C	3.14369500	1.09142600	0.13189900
C	2.72401600	2.46083800	0.19973700
C	1.40278300	2.75834700	0.03121500
H	1.89071100	-2.03841400	-0.43265800
C	2.61295000	-1.26234100	-0.22178700
C	4.50739600	0.73421700	0.24981600
H	3.46422100	3.23912500	0.36095900
H	1.03935800	3.78057000	0.04412400
C	4.91950000	-0.58423400	0.13872700
C	3.95784400	-1.58323400	-0.11095000
H	5.23374600	1.52484600	0.42194800
H	5.97026300	-0.84292900	0.22899500
H	4.26898400	-2.61796000	-0.22542800
N	0.80132300	0.37186100	-0.17090900
C	-1.62095000	-0.17638500	2.28889100
O	-0.92503200	0.76883400	2.52194100
O	-2.47890700	-0.95090700	2.61204000

**4**

Mn	0.92922800	-0.87788300	0.23457300
N	1.73879800	0.96016600	0.49617400
C	0.93119700	1.93300500	0.24769000
C	0.20758700	-2.35117300	-0.47501900
O	-0.19561700	-3.32940000	-0.96842200
C	0.68561500	-1.33389100	1.95323200
C	2.54018300	-1.63411200	0.15368100
O	0.55260300	-1.70273300	3.05343800
O	3.60092300	-2.11466700	0.10222900
O	1.44553700	3.18077800	0.19351300
C	2.85168800	3.04603400	0.58439300
C	3.09533200	1.51923800	0.59352300
H	2.96119500	3.50127600	1.57173300
H	3.45254800	3.58868500	-0.14537400
H	3.68706600	1.18496600	-0.26522500
H	3.59110700	1.17917300	1.50612100
C	-0.48142100	1.68046500	0.06488700
C	-2.15736700	0.06815800	0.13079000
C	-3.15137100	1.07240000	-0.12521900
C	-2.73416800	2.42190400	-0.28403000
C	-1.40489500	2.73001100	-0.15746300
H	-1.86713900	-2.01234800	0.63160700
C	-2.59770500	-1.25804500	0.37789100
C	-4.52133200	0.70451500	-0.18569800
H	-3.47427000	3.19261700	-0.47787400
H	-1.03945200	3.74746700	-0.23292700
C	-4.91376100	-0.60037200	0.02891300
C	-3.93941600	-1.58206900	0.32847800
H	-5.25598400	1.47778500	-0.39303800
H	-5.96372500	-0.87278000	-0.01503900
H	-4.24930400	-2.60349700	0.52863400
N	-0.81273400	0.38033900	0.16572500
C	1.24708400	-0.39899600	-1.95462000
O	0.87167300	0.74702300	-2.30201000
O	1.78754400	-1.27127900	-2.69059900

**5**

Mn	-0.70892300	0.63002800	1.17896100
N	-0.87565900	2.22748300	-0.07208400
C	-1.49976500	1.96947300	-1.16660200
C	-0.33268000	-0.93011500	1.97045500
O	-0.01566500	-1.92032800	2.49728000

C	-1.94295500	1.15699400	2.38529900
C	0.63815500	1.39115100	2.06384500
O	-2.69662900	1.48054700	3.21330900
O	1.51992400	1.90068300	2.62846800
O	-1.46616600	2.89483800	-2.14588500
C	-0.76257800	4.04929200	-1.57582500
C	-0.19258300	3.51844900	-0.24023800
H	-1.49939600	4.84455300	-1.44104800
H	-0.00285700	4.36083600	-2.29240100
H	0.88907600	3.35203400	-0.28376000
H	-0.40507400	4.18259100	0.60115600
C	-2.24619600	0.73248600	-1.31508900
C	-2.97433400	-1.19715200	-0.24416400
C	-3.72813800	-1.57422000	-1.40705200
C	-3.70154200	-0.72184800	-2.54206800
C	-2.98697700	0.44724500	-2.48583200
H	-2.56870600	-1.70520900	1.81600000
C	-3.08161700	-2.00903200	0.91511200
C	-4.50090600	-2.76589100	-1.38586700
H	-4.26584800	-0.99246300	-3.42958300
H	-2.96409300	1.14905800	-3.31105700
C	-4.56099900	-3.54792600	-0.25212200
C	-3.85558300	-3.15195000	0.91015300
H	-5.05399500	-3.04084200	-2.27961500
H	-5.15755700	-4.45481700	-0.24164200
H	-3.92824600	-3.75135900	1.81271100
N	-2.19013300	-0.06295800	-0.23567700
C	0.80334700	-0.03340600	-0.26427500
O	1.90982300	-0.51515600	0.18147900
O	0.54517400	0.09379700	-1.48497600
H	2.96743700	-0.97275100	-0.85401300
C	5.88116800	-0.93486100	-0.43845700
C	4.71298300	-1.89366400	-0.64456100
F	5.51550300	0.21913000	0.17804900
F	6.85012100	-1.50319500	0.33328900
F	6.47492600	-0.57548300	-1.60718200
O	3.71810400	-1.33565100	-1.45120300
H	5.13190700	-2.79327800	-1.11231100
H	4.34668800	-2.16477700	0.35442500

#### TS5\_6

Mn	-2.08070600	-1.50522700	-0.27108500
N	-1.94608700	-1.45112400	1.76617900
C	-1.98414200	-0.26603900	2.26066400

C	-1.88909800	-1.37716300	-2.04867900
O	-1.70769500	-1.35118100	-3.19806600
C	-3.79488100	-2.09166800	-0.32669100
C	-1.40330600	-3.15492900	-0.33527500
O	-4.87891400	-2.50624600	-0.39984900
O	-0.95246100	-4.22678500	-0.36039300
O	-1.68705800	-0.11459500	3.56386900
C	-1.48040000	-1.47133100	4.08595700
C	-1.48734200	-2.36471300	2.82312400
H	-2.30602600	-1.68456800	4.76818600
H	-0.53530300	-1.47515000	4.62853400
H	-0.49027100	-2.74026200	2.57033300
H	-2.16325300	-3.21851200	2.91535300
C	-2.37889900	0.86847200	1.43756600
C	-3.17299100	1.53416000	-0.64098000
C	-3.26233300	2.89382600	-0.18560900
C	-2.88071000	3.19134400	1.14762600
C	-2.46792400	2.17437100	1.97100100
H	-3.63637300	0.20587300	-2.28179500
C	-3.64098500	1.23273200	-1.94680900
C	-3.75308100	3.89698600	-1.06404600
H	-2.94139500	4.21417000	1.50727700
H	-2.19866000	2.34398200	3.00664500
C	-4.17308200	3.57492600	-2.33637500
C	-4.12902000	2.22693200	-2.76977000
H	-3.80069800	4.92141800	-0.70571200
H	-4.55083800	4.34532600	-3.00129200
H	-4.48871200	1.97006900	-3.76158000
N	-2.67533900	0.53995400	0.17257800
C	-0.06112600	-0.78322000	-0.19982300
O	0.80869600	-1.29569200	-1.04297600
O	0.27389200	0.09109000	0.62307500
H	1.95013800	-0.86178000	-0.97697100
C	4.81211000	-2.16265300	-0.61130100
C	3.89937000	-1.48279300	-1.62626500
F	4.12423900	-2.80273500	0.37095100
F	5.60587700	-3.09880500	-1.20595100
F	5.64605300	-1.28712500	0.01267900
O	3.09965400	-0.51686400	-1.02558300
H	4.56128000	-1.05881300	-2.39662900
H	3.31095900	-2.28493000	-2.09722500
C	4.11488600	3.10739800	0.61595800
C	4.72689500	2.36577800	-0.56789800
F	3.25915900	2.33589000	1.33451400

F	5.08232500	3.53095500	1.47618100
F	3.41678000	4.20957600	0.23743900
O	3.75297700	1.95442400	-1.48528100
H	3.48351100	1.00210600	-1.29112600
H	5.42288700	3.06377200	-1.04687100
H	5.30412200	1.52865300	-0.15622700

**6**

Mn	-0.97359900	-0.87305100	-0.21167800
N	-1.70531700	1.04495000	-0.31857500
C	-0.85258200	1.99355000	-0.17773400
C	-0.34898200	-2.51665700	0.16509500
O	-0.04195100	-3.59830700	0.45696200
C	-0.73478100	-1.02354200	-2.02182500
C	-2.61785500	-1.57866900	-0.30036600
O	-0.58719200	-1.14719200	-3.16287000
O	-3.68502000	-2.02636200	-0.37146500
O	-1.30775900	3.25407000	-0.14317800
C	-2.76460000	3.16584100	-0.33049800
C	-3.04760600	1.64399900	-0.38666300
H	-3.00227800	3.68787700	-1.25833000
H	-3.23148000	3.67065700	0.51528200
H	-3.64307700	1.29126500	0.45988500
H	-3.54543100	1.34258800	-1.31203200
C	0.57426900	1.70118000	-0.05965800
C	2.19811400	0.04595300	-0.07959300
C	3.22676300	1.03858800	0.08599700
C	2.84990200	2.39910400	0.17972700
C	1.52096400	2.73673600	0.09137500
H	1.83932700	-2.06387000	-0.38289900
C	2.59417700	-1.31018100	-0.22193200
C	4.58936100	0.63723600	0.13657100
H	3.61329700	3.16061200	0.30710800
H	1.18240200	3.76464000	0.13774300
C	4.93565000	-0.68934300	0.01036200
C	3.92545400	-1.66556000	-0.17975400
H	5.34962400	1.40135500	0.26944800
H	5.97783300	-0.99033800	0.04685900
H	4.20314300	-2.70859000	-0.29656200
N	0.86957600	0.39583100	-0.11976800
C	-1.11519600	-0.61779700	1.83632200
O	-2.40252300	-0.46785900	2.32473400
O	-0.20316100	-0.54632900	2.65834000
H	-2.33065300	-0.32218000	3.28911600



7

Mn	-0.94559000	-0.91414100	-0.19889800
N	-1.80015200	0.95744000	-0.42437700
C	-0.97671700	1.94405300	-0.19274600
C	-0.21390700	-2.51224500	0.15567600
O	0.15908600	-3.59094900	0.38938100
C	-0.72829800	-1.07923800	-1.99909200
C	-2.55247500	-1.68561600	-0.18493100
O	-0.58634500	-1.19008200	-3.14553000
O	-3.61252400	-2.16722800	-0.15939500
O	-1.54533000	3.18158300	-0.08612400
C	-2.94484400	3.00739100	-0.46060600
C	-3.16453400	1.48271900	-0.38444300
H	-3.07141100	3.39871300	-1.47528500
H	-3.55310500	3.58499200	0.23660400
H	-3.64988600	1.18077100	0.55257800
H	-3.76439900	1.11137300	-1.22109000
C	0.41785300	1.73492600	-0.03836900
C	2.15419300	0.13512300	-0.13152700
C	3.13613300	1.17209100	0.08795100
C	2.67710200	2.52587900	0.25987900
C	1.33475300	2.79190300	0.16787800
H	1.93444800	-1.96431200	-0.57972300
C	2.64173600	-1.17650400	-0.36449800
C	4.50538100	0.84378900	0.11046600
H	3.40038300	3.31828000	0.42966300
H	0.95135800	3.80413300	0.25075700
C	4.95047300	-0.46314700	-0.09449900
C	4.00432800	-1.46846500	-0.34266900
H	5.22243500	1.64306300	0.28586100
H	6.01158700	-0.69385200	-0.07354300
H	4.33005400	-2.48921800	-0.52637200
N	0.80461800	0.40242800	-0.12834400
C	-1.11446600	-0.56557300	1.84691700
O	-0.22720800	-1.26644100	2.65998900
O	-1.88245400	0.19578900	2.43802600
H	-0.40504300	-0.98339600	3.57894300

8

Mn	-0.44772100	-0.57592700	0.81256900
N	-0.02727900	1.44994300	0.82776300
C	-0.92845500	2.18957900	0.23584400
C	-0.72099400	-2.32812100	0.55699800

O	-0.78488300	-3.47770500	0.37910200
C	-1.28476800	-0.50292700	2.43046900
C	1.12735500	-0.96830900	1.55254200
O	-1.83157300	-0.46779200	3.45237300
O	2.14456600	-1.21856300	2.06028400
O	-0.66420900	3.52989900	0.19920300
C	0.70189200	3.67606500	0.69184500
C	0.98958300	2.33697900	1.39879400
H	0.73053000	4.54720300	1.34719700
H	1.35441500	3.83892100	-0.17223000
H	2.00130300	1.97618400	1.19717400
H	0.86228400	2.40932000	2.48869400
C	-2.12247600	1.63616800	-0.29201100
C	-3.47439800	-0.29661400	-0.40100100
C	-4.48981000	0.43973800	-1.11804700
C	-4.24558600	1.82594900	-1.42081500
C	-3.08441500	2.40953700	-0.98433500
H	-3.05525500	-2.20144000	0.52195500
C	-3.77340100	-1.64070100	-0.05872200
C	-5.68933200	-0.20036200	-1.48494700
H	-4.99458600	2.39470900	-1.96439400
H	-2.87909400	3.46112700	-1.15890000
C	-5.93978900	-1.53356800	-1.15740000
C	-4.97300300	-2.24413700	-0.43026200
H	-6.43269700	0.37579100	-2.03196900
H	-6.87213400	-2.00750700	-1.45009300
H	-5.15684700	-3.27685100	-0.14483100
N	-2.27553000	0.27694900	-0.04908400
C	0.31993200	-0.57715500	-1.11526700
O	1.71889500	-0.39184300	-1.24436800
O	-0.26276800	-0.72307600	-2.18439300
H	1.91268800	-0.42467200	-2.20221100
C	5.78529000	-0.46144800	-0.79827400
C	4.88062400	0.00951600	0.33445100
F	6.43936400	0.56183800	-1.40346500
F	6.73260500	-1.31960700	-0.33503700
F	5.09947200	-1.11409600	-1.77273900
O	3.91038700	0.92107300	-0.11848300
H	3.12547200	0.43613500	-0.45154900
H	4.44175700	-0.87949100	0.80040100
H	5.51903800	0.51021000	1.06800300

**TS8\_9**

Mn	0.66063000	0.78544300	0.80818200
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N	-0.02829000	-1.14568500	0.96784000
C	0.79904900	-2.05716900	0.52358300
C	1.16877900	2.50715500	0.60872100
O	1.38146000	3.64534400	0.53043400
C	1.57399200	0.60683300	2.38525800
C	-0.83222600	1.39657100	1.63060000
O	2.18443500	0.46623100	3.35324200
O	-1.75401500	1.76879500	2.21797200
O	0.39209100	-3.34719400	0.67850700
C	-0.99278100	-3.27786400	1.14137000
C	-1.16849900	-1.81607900	1.60172300
H	-1.11669900	-4.01665400	1.93370800
H	-1.63841500	-3.52893500	0.29418100
H	-2.11671000	-1.38925200	1.26147700
H	-1.10842600	-1.71616900	2.69437400
C	2.04289400	-1.71421600	-0.06219700
C	3.51803000	0.04765200	-0.63206700
C	4.46334800	-0.90758000	-1.15957000
C	4.13058100	-2.30688200	-1.11343000
C	2.93448500	-2.68994800	-0.56833400
H	3.20697600	2.15695700	-0.30257200
C	3.88543800	1.41430100	-0.69190200
C	5.68311000	-0.45897400	-1.70269300
H	4.83146700	-3.03634400	-1.50843000
H	2.64526800	-3.73439200	-0.51125800
C	6.01238200	0.89456800	-1.74714800
C	5.09950800	1.82799400	-1.23481100
H	6.37492400	-1.20244300	-2.09231000
H	6.95840400	1.21910000	-2.17012200
H	5.33419800	2.88894900	-1.25685800
N	2.31157600	-0.34862700	-0.09122300
C	-0.06461200	0.77066900	-1.04970800
O	-2.21528800	1.45199900	-0.92910800
O	0.02436900	0.58873300	-2.18511600
H	-2.35548000	1.60347800	-1.87466400
C	-6.05123700	0.02416400	-0.92056800
C	-5.00162100	0.25380800	0.16315700
F	-6.27163500	-1.29513200	-1.16953000
F	-7.25654600	0.55756700	-0.56647700
F	-5.71379500	0.58626100	-2.11225000
O	-3.77303000	-0.29601200	-0.17495600
H	-3.09073700	0.48323300	-0.52989200
H	-4.95741300	1.34301700	0.31767900
H	-5.41220400	-0.19788100	1.07842700

**9**

Mn	0.98708100	-0.94788300	0.03180800
N	1.87603900	0.89548900	-0.22083800
C	1.04053500	1.90109200	-0.08886300
C	0.22078000	-2.57132200	0.33417100
O	-0.15817400	-3.63936300	0.55959700
C	1.03425400	-0.61249300	1.87866000
C	2.61631900	-1.74899000	0.01641500
O	1.03943900	-0.37422600	2.99945700
O	3.66225200	-2.23456700	-0.00530100
O	1.60962800	3.13321600	-0.04905600
C	3.02427000	2.93620300	-0.36002100
C	3.24389600	1.42051300	-0.17599100
H	3.60544000	3.55841800	0.32059000
H	3.18524900	3.25981000	-1.39246300
H	3.86365800	0.99643300	-0.97100500
H	3.71604200	1.18499700	0.78741000
C	-0.35488900	1.69475300	0.01768300
C	-2.09567700	0.08565700	-0.06171000
C	-3.07491300	1.13243500	0.09546000
C	-2.62021100	2.49215000	0.22196200
C	-1.28014400	2.75904500	0.15313800
H	-1.87980100	-2.02783300	-0.45465600
C	-2.58084000	-1.22805700	-0.26825100
C	-4.44626500	0.81075800	0.09787800
H	-3.34867200	3.28851000	0.34104000
H	-0.89883000	3.77361900	0.20462900
C	-4.89057900	-0.49852100	-0.07172000
C	-3.94352000	-1.51458300	-0.26849800
H	-5.16256100	1.61863200	0.22800200
H	-5.95234600	-0.72548800	-0.06715700
H	-4.26839000	-2.53863300	-0.43109800
N	-0.74252200	0.35900000	-0.03012400
C	0.79299500	-1.05800500	-1.83362900
O	0.64841800	-1.06963700	-2.97018000

**10**

Mn	-0.57823100	-1.22922700	0.46003800
N	0.38415200	0.31331900	1.41223600
C	-0.14674600	1.47268100	1.26600900
C	-1.29674200	-2.46852600	-0.62867200
O	-1.66035100	-3.30047700	-1.35231700
C	-1.53916500	-1.72813300	1.93712100

C	0.71844100	-2.40289600	0.85898900
O	-2.15059600	-2.06908700	2.85758100
O	1.53739100	-3.17010500	1.14802100
O	0.49602600	2.53171100	1.77761500
C	1.73184800	2.00709900	2.38045600
C	1.63965900	0.47567800	2.16514000
H	1.73226700	2.30584500	3.42890300
H	2.56863600	2.47060000	1.85653600
H	2.47809200	0.08063900	1.58565500
H	1.57643000	-0.07976400	3.10564500
C	-1.43253600	1.62559100	0.58781600
C	-3.23013700	0.52081000	-0.37584000
C	-3.89036500	1.77737000	-0.61053300
C	-3.24270200	2.97016400	-0.20990600
C	-2.01981400	2.89652300	0.41213300
H	-3.46333600	-1.62624800	-0.50356900
C	-3.92038600	-0.67228100	-0.71809600
C	-5.17757200	1.79276500	-1.21339100
H	-3.72577900	3.92734700	-0.38171500
H	-1.49598400	3.77803300	0.76122200
C	-5.80917700	0.61676600	-1.55080900
C	-5.17525800	-0.62340800	-1.28685100
H	-5.65482100	2.75200900	-1.39119800
H	-6.79420000	0.63401600	-2.00625800
H	-5.68626700	-1.54942600	-1.53177600
N	-1.97880100	0.47009300	0.19011700
C	0.39295900	-0.54395700	-1.24051600
O	1.44137900	-1.33946100	-1.74089400
O	0.15692800	0.47283800	-1.87949200
H	1.72272300	-0.92667100	-2.58239800
C	4.94968600	0.79807500	-0.95117700
C	4.94243400	-0.72646700	-0.97896000
F	5.06261500	1.29429000	0.30631800
F	5.99350700	1.28849700	-1.66907000
F	3.81666000	1.32998700	-1.47870600
O	3.88824700	-1.25757900	-0.21274000
H	3.07128900	-1.30542100	-0.74783000
H	4.90597000	-1.03695500	-2.02921300
H	5.88951900	-1.06203200	-0.54795900

#### TS10\_11

Mn	1.02044100	1.59440900	-0.13940000
N	-0.58437400	1.38027000	1.11809000
C	-0.77077900	0.21286600	1.61686800

C	2.43885900	1.80661700	-1.25654300
O	3.31451600	2.03961900	-1.97390000
C	2.04786600	2.10147300	1.30806800
C	0.52673200	3.32215500	-0.50560800
O	2.69019000	2.40019900	2.21353900
O	0.25380400	4.41937000	-0.70002400
O	-1.79254100	0.03244800	2.44746800
C	-2.57998100	1.28101700	2.37946300
C	-1.64797900	2.26382100	1.63371400
H	-2.81334100	1.56435600	3.40636200
H	-3.46542600	1.04500500	1.78777800
H	-2.14272500	2.74996100	0.79027400
H	-1.19899000	3.02168800	2.28818100
C	0.14044100	-0.88618100	1.29511900
C	2.07438300	-1.53259900	0.18309300
C	1.89673000	-2.88401900	0.64266800
C	0.77738100	-3.18422800	1.45387400
C	-0.09991900	-2.18412900	1.79073900
H	3.37773500	-0.23355200	-0.95192000
C	3.21431500	-1.24288500	-0.61047500
C	2.84181100	-3.87977300	0.27705800
H	0.62216200	-4.20278400	1.79794000
H	-0.98086900	-2.35702800	2.39656500
C	3.93088400	-3.56455400	-0.50290100
C	4.11546100	-2.23125500	-0.94292100
H	2.68467300	-4.89576100	0.62821100
H	4.64863200	-4.33038600	-0.77971800
H	4.97865600	-1.98088300	-1.55210400
N	1.17172800	-0.54571300	0.51028300
C	0.00376000	0.89662800	-1.68314400
O	-1.97673000	2.22399400	-1.42984600
O	-0.24589700	0.31890300	-2.63788500
H	-2.38482100	2.57729600	-2.23013100
C	-3.28864700	-1.84633300	-0.89083300
C	-3.85409200	-0.45768200	-1.19411600
F	-3.53315000	-2.25521900	0.38436000
F	-3.82043600	-2.79900000	-1.71015000
F	-1.93405600	-1.91514800	-1.05338000
O	-3.33131800	0.51331600	-0.38017500
H	-2.65901400	1.40774200	-0.99376000
H	-3.64892700	-0.29959200	-2.27180600
H	-4.95102900	-0.57234200	-1.09508300

Mn	1.03400800	-0.90852900	-0.00008700
N	1.81364500	0.99244200	0.00035600
C	0.95826800	1.95177200	0.00030000
C	0.37301600	-2.61792200	-0.00065100
O	0.07127200	-3.72887600	-0.00102200
C	0.97889000	-0.85370500	1.88794000
C	2.71419400	-1.62332600	-0.00006900
O	0.93343600	-0.80859700	3.02884400
O	3.78020500	-2.05146900	-0.00005600
O	1.41742200	3.20090700	0.00091600
C	2.88874300	3.10325800	-0.00178700
C	3.16684000	1.57947500	0.00261700
H	3.24511000	3.61725900	0.89055000
H	3.24117500	3.61093800	-0.89936200
H	3.71720200	1.25041800	-0.88252400
H	3.71186100	1.25433400	0.89258200
C	-0.47878400	1.67578800	0.00001000
C	-2.13007900	0.03884200	-0.00005000
C	-3.14557500	1.06126700	-0.00002800
C	-2.75018300	2.41693200	-0.00005700
C	-1.41121500	2.72984300	-0.00005400
H	-1.81740200	-2.10349900	-0.00004900
C	-2.55168600	-1.31559900	-0.00003300
C	-4.51822600	0.69167000	0.00003900
H	-3.50538600	3.19664300	-0.00006900
H	-1.05680100	3.75312100	-0.00007500
C	-4.88820800	-0.63341100	0.00007800
C	-3.89097800	-1.64045400	0.00003700
H	-5.26499200	1.47982700	0.00007000
H	-5.93708700	-0.91143400	0.00014600
H	-4.18379900	-2.68562900	0.00006700
N	-0.79384100	0.37035500	-0.00000600
C	0.97948600	-0.85265100	-1.88812100
O	0.93444700	-0.80684200	-3.02901100