**Computational Prediction of Tc-99 NMR Chemical Shifts in Technetium Complexes with Radiopharmaceutical Applications**

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**DATA SHARING**

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**Input Model 1 – Geometry optimization (ADF 2019.3) - *trans*-[TcO2(en)2]+**

**SC-ZORA-B3LYP/TZP-ZORA/COSMO**

#!/bin/sh

"$ADFBIN/adf" <<eor

Atoms

1 Tc 3.467600000000 1.211600000000 3.753300000000 R=1.967

2 O 4.740400000000 0.048100000000 4.066300000000 R=1.517

3 O 2.176900000000 2.334900000000 3.430800000000 R=1.517

4 N 3.389400000000 1.682100000000 5.845000000000 R=1.608

5 N 2.021900000000 -0.283900000000 4.409400000000 R=1.608

6 N 3.600000000000 0.725400000000 1.672700000000 R=1.608

7 N 4.941000000000 2.665700000000 3.119300000000 R=1.608

8 C 2.971200000000 0.425800000000 6.556400000000 R=1.700

9 C 1.803200000000 -0.165400000000 5.876600000000 R=1.700

10 C 4.917200000000 1.244000000000 1.151000000000 R=1.700

11 C 5.067600000000 2.650100000000 1.671100000000 R=1.700

12 H 2.779800000000 2.276800000000 5.955600000000 R=1.350

13 H 4.177200000000 2.018600000000 5.998300000000 R=1.350

14 H 2.782700000000 0.697400000000 7.519300000000 R=1.350

15 H 3.803300000000 -0.352100000000 6.384100000000 R=1.350

16 H 1.591200000000 -1.074100000000 6.252900000000 R=1.350

17 H 1.074700000000 0.430300000000 5.917700000000 R=1.350

18 H 2.392200000000 -1.289800000000 4.116900000000 R=1.350

19 H 1.148200000000 -0.252600000000 3.832400000000 R=1.350

20 H 2.915000000000 1.122200000000 1.193700000000 R=1.350

21 H 3.519700000000 0.000000000000 1.650600000000 R=1.350

22 H 5.721000000000 0.629300000000 1.541500000000 R=1.350

23 H 4.906400000000 1.284200000000 0.000000000000 R=1.350

24 H 4.352800000000 3.130700000000 1.234800000000 R=1.350

25 H 5.772200000000 3.041300000000 1.283800000000 R=1.350

26 H 5.635000000000 2.448900000000 3.549400000000 R=1.350

27 H 4.669600000000 3.629200000000 3.490900000000 R=1.350

End

Basis

Type TZP

Core None

CreateOutput None

Tc ZORA/TZP/Tc

O ZORA/TZP/O

N ZORA/TZP/N

C ZORA/TZP/C

H ZORA/TZP/H

End

GUIBonds

1 1 3 2.0

2 1 2 2.0

3 1 6 1.0

4 1 7 1.0

5 1 5 1.0

6 4 12 1.0

7 4 13 1.0

8 4 8 1.0

9 5 19 1.0

10 5 18 1.0

11 6 21 1.0

12 6 20 1.0

13 7 26 1.0

14 7 27 1.0

15 8 14 1.0

16 8 15 1.0

17 8 9 1.0

18 9 17 1.0

19 9 16 1.0

20 10 22 1.0

21 10 23 1.0

22 10 11 1.0

23 11 25 1.0

24 11 24 1.0

End

NoPrint LOGFILE

XC

Hybrid B3LYP

End

Relativistic Scalar ZORA

Geometry

End

Symmetry NOSYM

Charge 1

SOLVATION

Surf Delley

Solv name=Water cav0=0.0 cav1=0.0067639

Charged method=CONJ

C-Mat POT

SCF VAR ALL

CSMRSP

END

NumericalQuality Good

eor

**Input Model 1 – NMR calculation (ADF 2019.3) - *trans*-[TcO2(en)2]+**

**SO-ZORA-SSB-D/TZ2P-ZORA/COSMO**

#!/bin/sh

"$ADFBIN/adf" <<eor

Atoms

1 Tc 3.567842000000 1.122673000000 3.758666000000 R=1.967

2 O 4.904593000000 0.005304000000 4.053078000000 R=1.517

3 O 2.229418000000 2.238158000000 3.463012000000 R=1.517

4 N 3.466106000000 1.570252000000 5.920221000000 R=1.608

5 N 2.134252000000 -0.413707000000 4.444344000000 R=1.608

6 N 3.669666000000 0.672856000000 1.597139000000 R=1.608

7 N 4.998808000000 2.659370000000 3.070968000000 R=1.608

8 C 2.829308000000 0.428512000000 6.637406000000 R=1.700

9 C 1.657827000000 -0.077853000000 5.817005000000 R=1.700

10 C 4.844350000000 1.367425000000 0.995871000000 R=1.700

11 C 4.948213000000 2.761733000000 1.584288000000 R=1.700

12 H 2.902179000000 2.408481000000 6.039439000000 R=1.350

13 H 4.372553000000 1.772741000000 6.332324000000 R=1.350

14 H 2.500325000000 0.726886000000 7.632468000000 R=1.350

15 H 3.582696000000 -0.350716000000 6.745863000000 R=1.350

16 H 1.200357000000 -0.943816000000 6.294563000000 R=1.350

17 H 0.900099000000 0.698628000000 5.718873000000 R=1.350

18 H 2.614810000000 -1.310108000000 4.456413000000 R=1.350

19 H 1.338356000000 -0.522446000000 3.822301000000 R=1.350

20 H 2.812250000000 1.011373000000 1.166797000000 R=1.350

21 H 3.717988000000 -0.321793000000 1.395886000000 R=1.350

22 H 5.730529000000 0.783821000000 1.242175000000 R=1.350

23 H 4.756260000000 1.414598000000 -0.089159000000 R=1.350

24 H 4.068050000000 3.349604000000 1.326297000000 R=1.350

25 H 5.828183000000 3.275942000000 1.198266000000 R=1.350

26 H 5.931129000000 2.378388000000 3.364923000000 R=1.350

27 H 4.831254000000 3.572394000000 3.484373000000 R=1.350

End

Basis

Type TZ2P

Core None

CreateOutput None

Tc ZORA/TZ2P/Tc

O ZORA/TZ2P/O

N ZORA/TZ2P/N

C ZORA/TZ2P/C

H ZORA/TZ2P/H

End

GUIBonds

1 1 2 2.0

2 1 3 2.0

3 1 7 1.0

4 1 6 1.0

5 1 5 1.0

6 4 13 1.0

7 4 12 1.0

8 4 8 1.0

9 5 19 1.0

10 5 18 1.0

11 6 21 1.0

12 6 20 1.0

13 7 27 1.0

14 7 26 1.0

15 8 15 1.0

16 8 14 1.0

17 8 9 1.0

18 9 17 1.0

19 9 16 1.0

20 10 22 1.0

21 10 23 1.0

22 10 11 1.0

23 11 24 1.0

24 11 25 1.0

End

Save TAPE10

NoPrint LOGFILE

XC

GGA SSB-D

End

Relativistic Spin-Orbit ZORA

Symmetry NOSYM

Charge 1

SOLVATION

Surf Delley

Solv name=Water cav0=0.0 cav1=0.0067639

Charged method=CONJ

C-Mat POT

SCF VAR ALL

CSMRSP

END

NumericalQuality Good

eor

# ===

# NMR

# ===

mkdir tapes

mv TAPE\* tapes 2>/dev/null

mv tapes/TAPE21 TAPE21 2>/dev/null

cp -f tapes/TAPE10 TAPE10

"$ADFBIN/nmr" <<eor

NMR

out iso tens

adfgui

ATOMS 1

u1k best

calc all

END

eor

mv TAPE21 tapes 2>/dev/null

rm -f TAPE\*

mv tapes/\* . 2>/dev/null

rm -r tapes

**Input Model 2 – Geometry optimization (GAUSSIAN 09 Rev. D.01) - *trans*-[TcO2(en)2]+**

**TPSS/def2-SVP/IEF-PCM(UFF)**

%mem=30Gb

%nproc=12

#TPSSTPSS/gen pseudo=read opt freq=noraman scrf=(iefpcm,read,solvent=water)

technetium

1 1

Tc 3.46760000 1.21160000 3.75330000

O 4.74040000 0.04810000 4.06630000

O 2.17690000 2.33490000 3.43080000

N 3.38940000 1.68210000 5.84500000

N 2.02190000 -0.28390000 4.40940000

N 3.60000000 0.72540000 1.67270000

N 4.94100000 2.66570000 3.11930000

C 2.97120000 0.42580000 6.55640000

C 1.80320000 -0.16540000 5.87660000

C 4.91720000 1.24400000 1.15100000

C 5.06760000 2.65010000 1.67110000

H 2.77980000 2.27680000 5.95560000

H 4.17720000 2.01860000 5.99830000

H 2.78270000 0.69740000 7.51930000

H 3.80330000 -0.35210000 6.38410000

H 1.59120000 -1.07410000 6.25290000

H 1.07470000 0.43030000 5.91770000

H 2.39220000 -1.28980000 4.11690000

H 1.14820000 -0.25260000 3.83240000

H 2.91500000 1.12220000 1.19370000

H 3.51970000 0.00000000 1.65060000

H 5.72100000 0.62930000 1.54150000

H 4.90640000 1.28420000 0.00000000

H 4.35280000 3.13070000 1.23480000

H 5.77220000 3.04130000 1.28380000

H 5.63500000 2.44890000 3.54940000

H 4.66960000 3.62920000 3.49090000

H 0

S 3 1.00

13.0107010 0.19682158D-01

1.9622572 0.13796524

0.44453796 0.47831935

S 1 1.00

0.12194962 1.0000000

P 1 1.00

0.8000000 1.0000000

\*\*\*\*

C 0

S 5 1.00

1238.4016938 0.54568832082D-02

186.29004992 0.40638409211D-01

42.251176346 0.18025593888

11.676557932 0.46315121755

3.5930506482 0.44087173314

S 1 1.00

0.40245147363 1.0000000

S 1 1.00

0.13090182668 1.0000000

P 3 1.00

9.4680970621 0.38387871728D-01

2.0103545142 0.21117025112

0.54771004707 0.51328172114

P 1 1.00

0.15268613795 1.0000000

D 1 1.00

0.8000000 1.0000000

\*\*\*\*

N 0

S 5 1.00

1712.8415853 -0.53934125305D-02

257.64812677 -0.40221581118D-01

58.458245853 -0.17931144990

16.198367905 -0.46376317823

5.0052600809 -0.44171422662

S 1 1.00

0.58731856571 1.0000000

S 1 1.00

0.18764592253 1.0000000

P 3 1.00

13.571470233 -0.40072398852D-01

2.9257372874 -0.21807045028

0.79927750754 -0.51294466049

P 1 1.00

0.21954348034 1.0000000

D 1 1.00

1.0000000 1.0000000

\*\*\*\*

O 0

S 5 1.00

2266.1767785 -0.53431809926D-02

340.87010191 -0.39890039230D-01

77.363135167 -0.17853911985

21.479644940 -0.46427684959

6.6589433124 -0.44309745172

S 1 1.00

0.80975975668 1.0000000

S 1 1.00

0.25530772234 1.0000000

P 3 1.00

17.721504317 0.43394573193D-01

3.8635505440 0.23094120765

1.0480920883 0.51375311064

P 1 1.00

0.27641544411 1.0000000

D 1 1.00

1.2000000 1.0000000

\*\*\*\*

Tc 0

S 3 1.00

7.4344020000 -1.1436289973

5.5513270000 1.8752000559

3.0230860000 0.23952854431

S 1 1.00

1.0647443990 1.0000000

S 1 1.00

0.48127808497 1.0000000

S 1 1.00

0.98299016952D-01 1.0000000

S 1 1.00

0.36659977936D-01 1.0000000

P 4 1.00

3.4490050000 -0.72277510434

2.6927370000 0.76458962802

0.94427370692 0.64533225171

0.41348148619 0.27195668811

P 1 1.00

0.15488152305 1.0000000

P 1 1.00

0.40300000000D-01 1.0000000

D 4 1.00

5.0906268699 -0.32176405405D-01

2.0156178510 0.21280802536

0.88113887240 0.44403309175

0.36427094833 0.40796933085

D 1 1.00

0.13678402297 1.0000000

F 1 1.00

0.7908500 1.0000000

\*\*\*\*

TC 0

TC-ECP 3 28

f potential

2

2 10.4000000 -26.56244747

2 5.2000000 -4.58568054

s-f potential

4

2 10.4223462 195.15916591

2 5.0365160 28.09260333

2 10.4000000 26.56244747

2 5.2000000 4.58568054

p-f potential

4

2 8.9504494 135.28456622

2 4.8544394 21.80650430

2 10.4000000 26.56244747

2 5.2000000 4.58568054

d-f potential

4

2 6.9456968 54.32972942

2 3.9705849 11.15506795

2 10.4000000 26.56244747

2 5.2000000 4.58568054

Radii=UFF

**Input Model 2 – NMR calculation (GAUSSIAN 09 Rev. D.01) – *trans*-[TcO2(en)2]+**

**B3LYP/NMR-DKH/IEF-PCM(UFF)**

%mem=30Gb

%nproc=12

#B3LYP/gen NMR=GIAO scrf=(iefpcm,read,solvent=water)

technetium

1 1

Tc 0.000036 -0.000378 0.000258

O -0.000882 -0.001352 -1.755833

O 0.000551 0.000287 1.756478

N 1.686236 1.398636 0.005994

N 1.687121 -1.398485 -0.006021

N -1.687188 -1.398442 0.007769

N -1.686337 1.398731 -0.005808

C 2.949102 0.680047 -0.346457

C 2.950105 -0.678554 0.344389

C -2.949208 -0.679049 -0.346384

C -2.949839 0.679923 0.343733

H 1.755756 1.790137 0.954643

H 1.549623 2.200464 -0.621462

H 3.837166 1.266377 -0.055530

H 2.963902 0.555631 -1.441529

H 3.838056 -1.264438 0.052300

H 2.966387 -0.553831 1.439358

H 1.756680 -1.791047 -0.954323

H 1.552482 -2.199936 0.622496

H -1.757454 -1.787874 0.957202

H -1.551565 -2.201916 -0.618082

H -2.962692 -0.555242 -1.441517

H -3.838018 -1.264625 -0.055989

H -2.967390 0.555748 1.438825

H -3.837351 1.266067 0.050390

H -1.755225 1.793959 -0.953075

H -1.549033 2.198032 0.624828

H 0

S 5 1.00

282.952156333090 0.00043

87.0622019486430 0.00051

26.7883698303517 0.00616

8.24257533241590 0.01303

2.53617702535874 0.09949

S 1 1.00

0.78036216164884 1.00000

S 1 1.00

0.24011143435349 1.00000

P 1 1.00

0.88150000000000 1.00000

P 1 1.00

0.17989200000000 1.00000

\*\*\*\*

C 0

S 6 1.00

8846.12353391750 0.00053

2948.70784463917 0.00077

982.902614879722 0.00405

327.634204959907 0.01403

109.211401653302 0.05345

36.4038005511008 0.17027

S 1 1.00

12.1346001837003 1.00000

S 1 1.00

4.04486672790009 1.00000

S 1 1.00

1.34828890930003 1.00000

S 1 1.00

0.44942963643334 1.00000

S 1 1.00

0.14980987881111 1.00000

P 4 1.00

37.2940933931704 0.00396

11.4751056594370 0.01889

3.53080174136525 0.09461

1.08640053580469 0.31889

P 1 1.00

0.33427708793991 1.00000

P 1 1.00

0.10285448859689 1.00000

D 1 1.00

0.47750000000000 1.00000

D 1 1.00

0.11998000000000 1.00000

\*\*\*\*

N 0

S 6 1.00

12238.3269689590 0.00056

4079.44232298633 0.00077

1359.81410766211 0.00406

453.271369220703 0.01391

151.090456406901 0.05299

50.3634854689670 0.16952

S 1 1.00

16.7878284896557 1.00000

S 1 1.00

5.59594282988522 1.00000

S 1 1.00

1.86531427662841 1.00000

S 1 1.00

0.62177142554280 1.00000

S 1 1.00

0.20725714184760 1.00000

P 4 1.00

54.1425482486954 0.00397

16.6592456149832 0.01954

5.12592172768714 0.09979

1.57720668544220 0.32845

P 1 1.00

0.48529436475145 1.00000

P 1 1.00

0.14932134300045 1.00000

D 1 1.00

0.47700000000000 1.00000

D 1 1.00

0.15026000000000 1.00000

\*\*\*\*

O 0

S 6 1.00

16178.1182314232 0.00060

5392.70607714106 0.00078

1797.56869238035 0.00410

599.189564126785 0.01388

199.729854708928 0.05277

66.5766182363094 0.16924

S 1 1.00

22.1922060787698 1.00000

S 1 1.00

7.39740202625660 1.00000

S 1 1.00

2.46580067541887 1.00000

S 1 1.00

0.82193355847296 1.00000

S 1 1.00

0.27397785282432 1.00000

P 4 1.00

73.8543986696091 0.00402

22.7244303598797 0.02013

6.99213241842453 0.10470

2.15142535951524 0.33605

P 1 1.00

0.66197703369700 1.00000

P 1 1.00

0.20368524113754 1.00000

D 1 1.00

0.92880000000000 1.00000

D 1 1.00

0.22975000000000 1.00000

\*\*\*\*

Tc 0

S 8 1.00

542008.175398728 0.00356

240892.522399434 0.00154

107063.343288638 0.00740

47583.7081282833 0.00442

21148.3147236815 0.01812

9399.25098830288 0.03066

4177.44488369017 0.07335

1856.64217052896 0.15043

S 1 1.00

825.174298012873 1.00000

S 1 1.00

366.744132450166 1.00000

S 1 1.00

162.997392200074 1.00000

S 1 1.00

72.4432854222550 1.00000

S 1 1.00

32.1970157432244 1.00000

S 1 1.00

14.3097847747664 1.00000

S 1 1.00

6.35990434434063 1.00000

S 1 1.00

2.82662415304028 1.00000

S 1 1.00

1.25627740135124 1.00000

S 1 1.00

0.55834551171166 1.00000

S 1 1.00

0.24815356076074 1.00000

S 1 1.00

0.11029047144922 1.00000

S 1 1.00

0.04901798731076 1.00000

S 1 1.00

0.00968256539472 1.00000

P 7 1.00

6996.64276548534 0.00240

2798.65710619414 0.00410

1119.46284247765 0.02062

447.785136991062 0.07310

179.114054796425 0.23151

71.6456219185699 0.46498

28.6582487674279 0.35270

P 1 1.00

11.4632995069712 1.00000

P 1 1.00

4.58531980278847 1.00000

P 1 1.00

1.83412792111539 1.00000

P 1 1.00

0.73365116844616 1.00000

P 1 1.00

0.29346046737846 1.00000

P 1 1.00

0.11738418695139 1.00000

P 1 1.00

0.04695367478055 1.00000

P 1 1.00

0.01878146991222 1.00000

D 4 1.00

521.281193644755 0.00351

124.755823975813 0.03202

45.3657541730230 0.14278

16.4966378810993 0.38792

D 1 1.00

5.99877741130882 1.00000

D 1 1.00

2.18137360411230 1.00000

D 1 1.00

0.79322676513175 1.00000

D 1 1.00

0.28844609641154 1.00000

D 1 1.00

0.10488948960420 1.00000

F 1 1.00

0.93440000000000 1.00000

F 1 1.00

0.26570000000000 1.00000

\*\*\*\*

Radii=UFF

**Model 1: Optimized structures at SC-ZORA-B3LYP/TZP-ZORA/COSMO level with ADF 2019.3 program.**

**a) Tc(0) complex**

Tc2(CO)10

22

Tc2C10O10

Tc 0.000024000 -0.000006000 1.583893000

Tc -0.000003000 -0.000009000 -1.583894000

C -1.875460000 -0.729610000 -1.456410000

C 0.729549000 -1.875490000 -1.456467000

C 1.875478000 0.729529000 -1.456391000

C -0.000029000 0.000115000 -3.540798000

C -0.729534000 -1.875481000 1.456445000

C 1.875491000 -0.729602000 1.456450000

C -0.000048000 0.000112000 3.540799000

C -1.875444000 0.729538000 1.456343000

C -0.729583000 1.875450000 -1.456325000

C 0.729606000 1.875453000 1.456353000

O -0.000048000 0.000203000 -4.688845000

O 1.142692000 -2.940655000 -1.405348000

O -2.940596000 -1.142826000 -1.405261000

O -1.142783000 2.940589000 -1.405134000

O 2.940645000 1.142664000 -1.405236000

O 1.142799000 2.940597000 1.405179000

O 2.940633000 -1.142803000 1.405321000

O -0.000100000 0.000199000 4.688845000

O -1.142681000 -2.940645000 1.405317000

O -2.940609000 1.142674000 1.405164000

**b) Tc(I) complexes**

*fac*-[Tc(ane-S3)(CO)3]+

28

TcC9H12S3O3

Tc 4.168118000 8.757003000 0.633322000

S 2.401980000 7.552105000 1.946737000

S 2.567254000 10.689697000 0.692780000

S 2.846188000 8.023873000 -1.373054000

O 5.980499000 6.236696000 0.512374000

O 6.167368000 10.349022000 -1.131215000

O 5.597663000 9.727061000 3.213863000

C 5.312608000 7.170968000 0.554400000

C 5.433188000 9.758781000 -0.472937000

C 5.073499000 9.361981000 2.258530000

C 1.434935000 8.962125000 2.630354000

H 0.517487000 8.550700000 3.051656000

H 2.049388000 9.321505000 3.454375000

C 1.230570000 6.878943000 0.674330000

H 0.852835000 5.940379000 1.076587000

H 0.395304000 7.570606000 0.600952000

C 1.875084000 6.624114000 -0.675169000

H 1.112789000 6.362166000 -1.409024000

H 2.592770000 5.806335000 -0.631026000

C 1.531295000 9.317869000 -1.582230000

H 1.354507000 9.399555000 -2.653365000

H 0.622428000 8.937680000 -1.123054000

C 1.916661000 10.677899000 -1.030842000

H 1.056544000 11.347231000 -1.055394000

H 2.714269000 11.137080000 -1.612792000

C 1.102587000 10.072911000 1.651518000

H 0.716214000 10.931087000 2.198642000

H 0.346617000 9.768295000 0.932293000

*trans-*TcCl(CO)3(PPh3)2

76

TcC39P2H30O3Cl

Tc 0.005707000 -0.024194000 -0.192593000

C -0.037153000 -0.652079000 -1.993762000

C 0.010420000 -1.890113000 0.530984000

O -0.000866000 -2.974726000 0.904459000

O -0.068457000 -0.979518000 -3.107766000

Cl 0.100331000 1.124797000 2.107997000

P 2.520501000 -0.007043000 -0.051552000

C 3.252936000 1.633686000 0.365563000

C 3.157230000 2.687542000 -0.552077000

C 3.853611000 1.873109000 1.604380000

C 3.661732000 3.945962000 -0.242748000

H 2.700450000 2.531425000 -1.520571000

C 4.350631000 3.136713000 1.916799000

H 3.937216000 1.079772000 2.333411000

C 4.257626000 4.175356000 0.996011000

H 3.586073000 4.746096000 -0.968775000

H 4.810047000 3.304871000 2.883223000

H 4.646470000 5.156490000 1.239349000

C 3.252652000 -1.135848000 1.221977000

C 4.493405000 -1.750532000 1.011222000

C 2.588699000 -1.357357000 2.433543000

C 5.051109000 -2.572350000 1.986668000

H 5.030676000 -1.596308000 0.085778000

C 3.150470000 -2.177465000 3.408780000

H 1.640721000 -0.872446000 2.624453000

C 4.381356000 -2.788891000 3.188056000

H 6.009965000 -3.042048000 1.804141000

H 2.623340000 -2.336574000 4.341681000

H 4.815804000 -3.429838000 3.945563000

C 3.416388000 -0.535097000 -1.579940000

C 4.508924000 0.162004000 -2.105194000

C 3.015311000 -1.723404000 -2.203060000

C 5.170566000 -0.307279000 -3.238593000

H 4.856317000 1.070159000 -1.634530000

C 3.682752000 -2.197166000 -3.327145000

H 2.182426000 -2.291389000 -1.809666000

C 4.759440000 -1.485649000 -3.852853000

H 6.011714000 0.249238000 -3.633202000

H 3.358940000 -3.119234000 -3.793680000

H 5.274514000 -1.849506000 -4.733321000

C -0.009619000 1.854612000 -0.906312000

O -0.024358000 2.916953000 -1.329862000

P -2.504267000 -0.040336000 -0.024535000

C -3.387801000 -1.575912000 -0.571171000

C -4.724091000 -1.777739000 -0.196292000

C -2.766748000 -2.539044000 -1.369518000

C -5.415807000 -2.909249000 -0.612222000

H -5.230886000 -1.052490000 0.425796000

C -3.459997000 -3.674602000 -1.786858000

H -1.739621000 -2.417573000 -1.675727000

C -4.784826000 -3.862930000 -1.409443000

H -6.446789000 -3.046789000 -0.310161000

H -2.958575000 -4.409144000 -2.404851000

H -5.322798000 -4.746401000 -1.730369000

C -3.208223000 0.165933000 1.671440000

C -4.262382000 1.035292000 1.963824000

C -2.704895000 -0.648930000 2.692354000

C -4.796956000 1.092879000 3.250285000

H -4.682130000 1.668518000 1.195385000

C -3.246808000 -0.601191000 3.970720000

H -1.884626000 -1.325439000 2.496748000

C -4.292177000 0.275822000 4.256112000

H -5.612018000 1.775181000 3.458642000

H -2.845206000 -1.240916000 4.747040000

H -4.708597000 0.320177000 5.255050000

C -3.308642000 1.278855000 -1.030385000

C -3.158496000 2.620548000 -0.654781000

C -4.000714000 0.981492000 -2.208221000

C -3.709838000 3.637128000 -1.426540000

H -2.615531000 2.878061000 0.246150000

C -4.541067000 2.002899000 -2.987189000

H -4.127358000 -0.044772000 -2.524472000

C -4.402285000 3.331236000 -2.596666000

H -3.594047000 4.667832000 -1.115074000

H -5.073937000 1.754546000 -3.896875000

H -4.828308000 4.123746000 -3.199575000

*trans-*TcCl(CO)3(PMe2Ph)2

48

TcC19P2H22O3Cl

Tc 0.027561000 0.180685000 0.278617000

C 0.991207000 1.791373000 -0.060637000

C -0.199085000 -0.135095000 -1.683054000

O -0.320245000 -0.296563000 -2.813310000

O 1.580219000 2.773194000 -0.259378000

Cl -1.206557000 -2.024771000 0.816595000

P 2.050937000 -1.251543000 0.292965000

C 3.643606000 -0.436080000 -0.126148000

C 4.660135000 -0.251515000 0.816235000

C 3.835790000 0.047559000 -1.427127000

C 5.844182000 0.394500000 0.463010000

H 4.543786000 -0.609097000 1.830302000

C 5.020605000 0.683111000 -1.781227000

H 3.060073000 -0.068385000 -2.174569000

C 6.029272000 0.860087000 -0.835137000

H 6.620586000 0.529769000 1.205925000

H 5.154353000 1.044363000 -2.793457000

H 6.950904000 1.358785000 -1.109044000

C 0.220795000 0.448326000 2.256270000

O 0.328038000 0.598697000 3.387676000

P -2.141660000 1.370222000 0.302738000

C -3.611156000 0.393200000 -0.204323000

C -4.407207000 -0.255536000 0.745277000

C -3.918930000 0.236972000 -1.561025000

C -5.493935000 -1.029879000 0.348137000

H -4.187556000 -0.166155000 1.800640000

C -5.005089000 -0.538275000 -1.957435000

H -3.318518000 0.719895000 -2.321714000

C -5.796658000 -1.173334000 -1.003301000

H -6.101955000 -1.522515000 1.097252000

H -5.231960000 -0.643543000 -3.011471000

H -6.642457000 -1.775880000 -1.311285000

C -2.209040000 2.840459000 -0.796325000

H -1.459275000 3.556371000 -0.458738000

H -1.973876000 2.562855000 -1.822688000

H -3.195214000 3.304008000 -0.761565000

C -2.629422000 2.092735000 1.917832000

H -3.599750000 2.584346000 1.845545000

H -2.667213000 1.324597000 2.688404000

H -1.873432000 2.825346000 2.201869000

C 2.366233000 -2.099095000 1.886634000

H 2.532440000 -1.377517000 2.684978000

H 1.474158000 -2.677481000 2.125568000

H 3.225025000 -2.766667000 1.812733000

C 1.986170000 -2.665210000 -0.877563000

H 1.085366000 -3.239341000 -0.662780000

H 1.935922000 -2.304739000 -1.903963000

H 2.868031000 -3.295575000 -0.760068000

*cis-*TcCl(CO)3(PMe2Ph)2

48

TcC19P2H22O3Cl

Tc 0.010693000 -0.702612000 0.022357000

C 0.379939000 -0.513981000 1.890632000

C -1.345044000 -2.074598000 0.404788000

C 1.375597000 -2.104929000 -0.184458000

O -2.108958000 -2.899237000 0.642812000

O 0.588933000 -0.413990000 3.027410000

O 2.154794000 -2.940661000 -0.307888000

Cl -0.544942000 -0.928611000 -2.489153000

P 1.807156000 1.010226000 -0.557113000

P -1.791221000 1.082703000 0.137567000

C 3.505734000 0.472509000 -0.095170000

C 4.469525000 0.143721000 -1.052658000

C 3.844258000 0.379928000 1.261595000

C 5.745569000 -0.259115000 -0.662034000

H 4.241236000 0.201412000 -2.108339000

C 5.118886000 -0.016877000 1.649688000

H 3.117168000 0.620130000 2.027394000

C 6.074849000 -0.337569000 0.687395000

H 6.481522000 -0.505951000 -1.417333000

H 5.364761000 -0.074898000 2.703004000

H 7.068047000 -0.646734000 0.989245000

C -3.520299000 0.454176000 0.119160000

C -4.402592000 0.646355000 1.186638000

C -3.970683000 -0.231282000 -1.017475000

C -5.712390000 0.174213000 1.113334000

H -4.087180000 1.166757000 2.080515000

C -5.279468000 -0.695024000 -1.090228000

H -3.293706000 -0.409766000 -1.844154000

C -6.155674000 -0.491195000 -0.025496000

H -6.385063000 0.333692000 1.947325000

H -5.613904000 -1.217456000 -1.978127000

H -7.175490000 -0.851475000 -0.083402000

C 1.938499000 1.455326000 -2.328449000

H 2.069717000 0.561763000 -2.934801000

H 1.004012000 1.923763000 -2.633216000

H 2.763549000 2.149543000 -2.489126000

C 1.748548000 2.668654000 0.246585000

H 0.854761000 3.206206000 -0.065311000

H 1.734753000 2.565921000 1.330516000

H 2.625598000 3.246955000 -0.044616000

C -1.734238000 2.172223000 1.613837000

H -1.808165000 1.580964000 2.525600000

H -0.778624000 2.693492000 1.625435000

H -2.537229000 2.909025000 1.589519000

C -1.839194000 2.286568000 -1.253519000

H -0.935099000 2.893246000 -1.255887000

H -1.895378000 1.742295000 -2.194279000

H -2.705488000 2.940292000 -1.150121000

*trans-*TcBr(CO)3(PPh3)2

76

TcC39P2H30O3Br

Tc 0.004315000 0.199578000 -0.153861000

C -0.000829000 1.975446000 -0.811866000

C -0.019174000 0.967725000 1.685241000

O -0.024095000 1.514398000 2.694960000

O -0.013495000 3.050216000 -1.246200000

P -2.509461000 0.086839000 -0.097102000

C -3.255778000 -1.252725000 -1.121262000

C -3.070289000 -1.246334000 -2.509708000

C -3.964677000 -2.308919000 -0.542466000

C -3.592244000 -2.264527000 -3.299921000

H -2.527618000 -0.441219000 -2.987104000

C -4.480645000 -3.332646000 -1.334597000

H -4.117215000 -2.342664000 0.526884000

C -4.297526000 -3.313555000 -2.713349000

H -3.446005000 -2.238150000 -4.372704000

H -5.026008000 -4.144165000 -0.868466000

H -4.700046000 -4.109257000 -3.328083000

C -3.280037000 -0.166701000 1.568055000

C -4.563041000 0.326210000 1.840593000

C -2.607995000 -0.881374000 2.564276000

C -5.153096000 0.115504000 3.082860000

H -5.106862000 0.881124000 1.088225000

C -3.201067000 -1.093274000 3.806616000

H -1.628975000 -1.293753000 2.364145000

C -4.472741000 -0.593621000 4.070380000

H -6.143910000 0.507164000 3.277402000

H -2.666174000 -1.650669000 4.566003000

H -4.931383000 -0.755436000 5.038328000

C -3.359137000 1.633541000 -0.650979000

C -4.339604000 1.665950000 -1.645954000

C -3.019661000 2.827638000 -0.001836000

C -4.955188000 2.868199000 -1.993113000

H -4.638000000 0.759262000 -2.152071000

C -3.641951000 4.023032000 -0.339626000

H -2.271158000 2.830418000 0.780523000

C -4.609467000 4.047887000 -1.342736000

H -5.710865000 2.875009000 -2.769236000

H -3.368033000 4.934446000 0.177110000

H -5.090582000 4.980155000 -1.611797000

C 0.086501000 -0.431687000 -2.054714000

O 0.170810000 -0.735194000 -3.155244000

P 2.509916000 0.144600000 -0.021214000

C 3.202229000 1.854511000 0.000051000

C 3.647639000 2.439709000 1.189979000

C 3.182780000 2.630389000 -1.166056000

C 4.071664000 3.766760000 1.210462000

H 3.669057000 1.866561000 2.106630000

C 3.619287000 3.950301000 -1.146795000

H 2.827777000 2.208816000 -2.097986000

C 4.064360000 4.523545000 0.042685000

H 4.411343000 4.203890000 2.141410000

H 3.605635000 4.531762000 -2.060218000

H 4.399607000 5.553284000 0.058791000

C 3.293522000 -0.628178000 1.467981000

C 4.686001000 -0.786674000 1.511111000

C 2.537073000 -1.035510000 2.567867000

C 5.302929000 -1.323171000 2.634729000

H 5.296244000 -0.489182000 0.668641000

C 3.155845000 -1.573469000 3.695524000

H 1.461036000 -0.963413000 2.542485000

C 4.538431000 -1.716038000 3.732706000

H 6.380072000 -1.435227000 2.652338000

H 2.552811000 -1.885478000 4.539320000

H 5.019609000 -2.135101000 4.607999000

C 3.416915000 -0.716413000 -1.383255000

C 2.970718000 -1.988234000 -1.762057000

C 4.569392000 -0.198280000 -1.983778000

C 3.658066000 -2.721930000 -2.723448000

H 2.090090000 -2.412446000 -1.295781000

C 5.253495000 -0.933748000 -2.949834000

H 4.945675000 0.775302000 -1.703106000

C 4.800482000 -2.195720000 -3.322386000

H 3.299130000 -3.704758000 -3.003394000

H 6.143589000 -0.517535000 -3.405783000

H 5.334422000 -2.766225000 -4.072669000

Br -0.040678000 -2.446854000 0.507592000

*cis-*TcBr(CO)3(PPh3)2

76

TcC39P2H30O3Br

Tc 0.013560000 -0.681988000 -1.401724000

C -0.164487000 0.911248000 -2.435170000

C 1.349603000 -1.295541000 -2.651493000

C -1.269029000 -1.599953000 -2.527742000

O 2.080292000 -1.640620000 -3.470876000

O -0.297045000 1.833558000 -3.121815000

O -1.945733000 -2.204433000 -3.232635000

P -2.113786000 0.197971000 0.015017000

P 2.085462000 0.166938000 0.032709000

C -3.675215000 -0.210160000 -0.895700000

C -4.671286000 -1.034619000 -0.367831000

C -3.859726000 0.336343000 -2.173056000

C -5.823544000 -1.312507000 -1.102330000

H -4.565294000 -1.460653000 0.619151000

C -5.012323000 0.065598000 -2.900147000

H -3.109377000 0.986784000 -2.604936000

C -5.998411000 -0.763800000 -2.367693000

H -6.584528000 -1.954038000 -0.675074000

H -5.139974000 0.501421000 -3.883188000

H -6.895434000 -0.977904000 -2.935766000

C 3.663460000 -0.648855000 -0.494922000

C 4.798097000 0.065767000 -0.888246000

C 3.729031000 -2.047416000 -0.442474000

C 5.972282000 -0.604562000 -1.229109000

H 4.782657000 1.145624000 -0.925971000

C 4.903261000 -2.712282000 -0.775765000

H 2.860125000 -2.618068000 -0.140437000

C 6.029166000 -1.993095000 -1.172984000

H 6.842165000 -0.034646000 -1.531899000

H 4.937174000 -3.793804000 -0.725729000

H 6.943101000 -2.512250000 -1.434457000

Br 0.159427000 -3.014010000 -0.040242000

C -2.475867000 -0.379307000 1.736155000

C -2.465473000 -1.753238000 2.013056000

C -2.767353000 0.513695000 2.774559000

C -2.756468000 -2.219976000 3.291480000

H -2.216912000 -2.461792000 1.236017000

C -3.051218000 0.042814000 4.054684000

H -2.774505000 1.579373000 2.596725000

C -3.050516000 -1.324091000 4.316437000

H -2.747844000 -3.285509000 3.485659000

H -3.273937000 0.749679000 4.844483000

H -3.273404000 -1.688563000 5.311833000

C -2.247882000 2.032986000 0.162416000

C -3.492090000 2.675353000 0.228810000

C -1.088367000 2.802481000 0.267305000

C -3.565329000 4.054157000 0.395015000

H -4.406602000 2.102691000 0.153725000

C -1.161045000 4.183073000 0.437806000

H -0.117857000 2.331702000 0.210670000

C -2.400161000 4.811921000 0.499792000

H -4.533913000 4.536347000 0.443877000

H -0.249349000 4.761744000 0.515457000

H -2.460223000 5.885829000 0.626346000

C 2.144698000 -0.096833000 1.857458000

C 3.366174000 -0.174913000 2.540434000

C 0.958918000 -0.165602000 2.587465000

C 3.390939000 -0.305780000 3.925060000

H 4.300416000 -0.131915000 1.997305000

C 0.982910000 -0.292092000 3.974901000

H 0.008714000 -0.134672000 2.078654000

C 2.199162000 -0.360604000 4.646206000

H 4.341752000 -0.362888000 4.440579000

H 0.051233000 -0.342447000 4.523807000

H 2.220965000 -0.461798000 5.724430000

C 2.469136000 1.966688000 -0.144063000

C 2.617776000 2.812564000 0.959946000

C 2.606213000 2.508233000 -1.429425000

C 2.903797000 4.164931000 0.782448000

H 2.512322000 2.425604000 1.963511000

C 2.904735000 3.854767000 -1.604490000

H 2.497019000 1.878038000 -2.302807000

C 3.052945000 4.688687000 -0.497645000

H 3.013739000 4.804718000 1.649553000

H 3.019313000 4.251760000 -2.605299000

H 3.281714000 5.738478000 -0.633950000

*cis*-TcBr(CO)3(PMe2Ph)2

48

TcC19P2H22O3Br

Tc -0.045148000 -0.022311000 -0.717938000

C -0.405586000 1.731776000 -1.387366000

C 1.332361000 -0.318993000 -2.087540000

C -1.398925000 -0.828428000 -1.895770000

O 2.118210000 -0.495028000 -2.907106000

O -0.617908000 2.791915000 -1.807570000

O -2.169258000 -1.309488000 -2.599815000

P -1.841170000 0.265359000 1.068402000

P 1.753097000 0.866437000 0.839733000

C -3.562069000 0.264565000 0.413958000

C -4.452832000 -0.782575000 0.668235000

C -3.996108000 1.344931000 -0.365509000

C -5.752152000 -0.743252000 0.165003000

H -4.150468000 -1.633794000 1.262607000

C -5.294421000 1.385711000 -0.861615000

H -3.326304000 2.167012000 -0.586570000

C -6.177834000 0.340820000 -0.595761000

H -6.430737000 -1.560868000 0.375011000

H -5.615737000 2.233881000 -1.453515000

H -7.189898000 0.373215000 -0.979832000

C 3.483542000 0.498224000 0.336596000

C 4.308806000 1.476217000 -0.227705000

C 3.992301000 -0.794726000 0.517727000

C 5.620244000 1.172927000 -0.587063000

H 3.946516000 2.482837000 -0.385324000

C 5.303908000 -1.092703000 0.163906000

H 3.363917000 -1.573608000 0.930239000

C 6.122945000 -0.109131000 -0.387578000

H 6.247701000 1.943764000 -1.017489000

H 5.685311000 -2.094280000 0.319873000

H 7.145308000 -0.341426000 -0.659875000

C -1.886581000 -0.977498000 2.413724000

H -1.986852000 -1.978503000 2.000424000

H -0.943758000 -0.939059000 2.956033000

H -2.707911000 -0.766134000 3.098614000

C -1.836191000 1.848058000 2.015352000

H -0.936963000 1.912288000 2.626038000

H -1.857120000 2.698107000 1.335092000

H -2.707836000 1.890715000 2.668540000

C 1.756129000 2.690138000 1.062200000

H 1.834108000 3.192632000 0.099443000

H 0.814381000 2.988450000 1.520028000

H 2.579110000 3.002880000 1.704934000

C 1.739709000 0.264923000 2.578889000

H 0.847821000 0.629151000 3.086651000

H 1.726958000 -0.823320000 2.590945000

H 2.620506000 0.630398000 3.106514000

Br 0.503140000 -2.525168000 0.221686000

[Tc(CH3NC)6]+

37

TcC12N6H18

Tc 0.005477000 0.001640000 0.001484000

C -1.283837000 1.132953000 1.151344000

C 0.420229000 1.651361000 -1.171244000

C 1.570021000 0.499099000 1.255192000

C -0.412523000 -1.643733000 1.178981000

C -1.555351000 -0.496135000 -1.255648000

C 1.287133000 -1.136374000 -1.151385000

N -2.017545000 1.763307000 1.803035000

N 2.455451000 0.776902000 1.961886000

N -0.654414000 -2.566878000 1.849504000

N 2.009626000 -1.775583000 -1.807141000

N 0.656846000 2.580475000 -1.835429000

N -2.436199000 -0.774746000 -1.967575000

C -2.911459000 2.530590000 2.602574000

H -3.357095000 3.319302000 1.998081000

H -3.698691000 1.886102000 2.991462000

H -2.366764000 2.976255000 3.433684000

C -3.511898000 -1.111989000 -2.836947000

H -3.925675000 -0.204167000 -3.273890000

H -3.149305000 -1.762252000 -3.631782000

H -4.288146000 -1.628028000 -2.273644000

C 0.945435000 3.716235000 -2.644652000

H 1.603468000 4.393482000 -2.102189000

H 1.434982000 3.395288000 -3.562857000

H 0.019155000 4.233255000 -2.891050000

C 2.888551000 -2.555758000 -2.611539000

H 3.921258000 -2.304358000 -2.373292000

H 2.720037000 -3.613751000 -2.416268000

H 2.700445000 -2.348221000 -3.664054000

C 3.538130000 1.113083000 2.823412000

H 3.609865000 0.377295000 3.623189000

H 4.467491000 1.121086000 2.255886000

H 3.369458000 2.099144000 3.253744000

C -0.952350000 -3.693794000 2.667355000

H -0.040107000 -4.256826000 2.859488000

H -1.374761000 -3.357259000 3.613045000

H -1.671405000 -4.334196000 2.158423000

[Tc(tert.BuNC)6]+

91

TcC30N6H54

Tc 0.012310000 0.004164000 -0.016174000

C -1.312262000 -0.039702000 -1.600435000

C 1.133735000 -1.494649000 -0.889295000

C 1.139924000 1.425677000 -1.002114000

C -1.106921000 1.495695000 0.869890000

C -1.125999000 -1.411290000 0.964150000

C 1.331379000 0.047990000 1.573048000

N -2.065605000 -0.061160000 -2.492818000

N 1.778027000 2.229305000 -1.559942000

N -1.748042000 2.331542000 1.373864000

N 2.074665000 0.068052000 2.473790000

N 1.776889000 -2.341660000 -1.372023000

N -1.779927000 -2.205909000 1.516560000

C -3.013639000 -0.079634000 -3.587362000

C -2.603265000 -3.180727000 2.199877000

C 2.568297000 -3.403077000 -1.958011000

C 3.000526000 0.088527000 3.587276000

C 2.578068000 3.219283000 -2.249868000

C -2.542963000 3.366496000 2.000166000

C 3.440492000 -2.792783000 -3.065816000

H 4.108782000 -2.034607000 -2.656655000

H 4.044389000 -3.576370000 -3.524660000

H 2.820979000 -2.335076000 -3.837591000

C 1.606060000 -4.452368000 -2.535770000

H 2.181757000 -5.264423000 -2.981184000

H 0.970050000 -4.866886000 -1.753089000

H 0.972517000 -4.012847000 -3.306659000

C 3.440987000 -4.014387000 -0.850869000

H 4.102599000 -3.262290000 -0.420328000

H 2.821613000 -4.433023000 -0.057116000

H 4.051707000 -4.813685000 -1.272156000

C -2.383680000 -4.546061000 1.530033000

H -2.669381000 -4.511397000 0.478333000

H -1.337988000 -4.846645000 1.600080000

H -2.994979000 -5.297231000 2.031338000

C -2.171892000 -3.219781000 3.674090000

H -2.302560000 -2.242969000 4.140718000

H -2.783547000 -3.945296000 4.211233000

H -1.125910000 -3.514115000 3.763424000

C -4.069859000 -2.740330000 2.071424000

H -4.710639000 -3.461853000 2.579283000

H -4.221477000 -1.761252000 2.526845000

H -4.367574000 -2.689222000 1.023702000

C -2.957522000 -1.466845000 -4.245543000

H -1.961523000 -1.666511000 -4.641461000

H -3.212359000 -2.246485000 -3.527187000

H -3.672584000 -1.506143000 -5.068095000

C -2.611487000 1.015407000 -4.587443000

H -3.315517000 1.019553000 -5.420466000

H -2.628888000 1.997398000 -4.113800000

H -1.610988000 0.832314000 -4.979863000

C -4.411495000 0.194198000 -3.011366000

H -4.685003000 -0.568447000 -2.281748000

H -4.445797000 1.170815000 -2.527605000

H -5.144922000 0.181165000 -3.818415000

C 3.364337000 -1.364358000 3.931440000

H 2.475965000 -1.928027000 4.217603000

H 3.833515000 -1.857764000 3.079827000

H 4.065134000 -1.373750000 4.766906000

C 4.247407000 0.877361000 3.156790000

H 3.983765000 1.901859000 2.892175000

H 4.961080000 0.904674000 3.980925000

H 4.726287000 0.405418000 2.298385000

C 2.305308000 0.772144000 4.774965000

H 2.987458000 0.800618000 5.625455000

H 2.024124000 1.794948000 4.521956000

H 1.409245000 0.224070000 5.067098000

C -3.458526000 3.979170000 0.929134000

H -2.869989000 4.419958000 0.124029000

H -4.119965000 3.222268000 0.506643000

H -4.069880000 4.761375000 1.380444000

C -3.371129000 2.718797000 3.120768000

H -4.033583000 1.952594000 2.716913000

H -2.721175000 2.262357000 3.867749000

H -3.979472000 3.481054000 3.608851000

C -1.585690000 4.424616000 2.570017000

H -0.919498000 3.983240000 3.311695000

H -0.982827000 4.868638000 1.777381000

H -2.164292000 5.214688000 3.049969000

C 1.927958000 4.594976000 -2.035922000

H 0.915755000 4.612032000 -2.440678000

H 1.886103000 4.841778000 -0.974696000

H 2.518586000 5.356594000 -2.546189000

C 2.604486000 2.855938000 -3.742250000

H 3.041775000 1.868667000 -3.893194000

H 1.597013000 2.860138000 -4.159168000

H 3.205993000 3.587839000 -4.282356000

C 3.994024000 3.186342000 -1.653834000

H 3.971202000 3.424276000 -0.589928000

H 4.444963000 2.202168000 -1.783503000

H 4.617652000 3.923243000 -2.160968000

[Tc(CO)3(H2O)2Cl]

14

TcC3H4O5Cl

Tc -0.030726000 -0.080482000 -0.004814000

O 0.862791000 -1.442867000 1.572461000

H 0.891491000 -2.368291000 1.279574000

O 0.931774000 -1.637136000 -1.334397000

H 0.494471000 -1.808928000 -2.182844000

H 1.796271000 -1.170883000 1.632689000

H 1.813185000 -1.291550000 -1.561948000

C -0.671304000 1.173926000 1.293883000

C -1.734983000 -0.979140000 0.012141000

C -0.640493000 1.079772000 -1.401296000

O -1.037735000 1.926461000 2.086798000

O -0.992648000 1.783354000 -2.244746000

O -2.751871000 -1.523263000 0.022670000

Cl 2.354699000 0.773409000 -0.010612000

[Tc(CO)3(H2O)2Br]

14

TcC3H4O5Br

Tc -0.383338000 -0.104926000 -0.000065000

O 0.166340000 -1.636681000 1.585720000

H 0.005081000 -2.539774000 1.266543000

O 0.195761000 -1.854115000 -1.321329000

H -0.301523000 -1.950822000 -2.148456000

H 1.133963000 -1.578662000 1.682853000

H 1.122817000 -1.726521000 -1.589360000

C -0.742653000 1.268795000 1.284363000

C -2.238809000 -0.626662000 0.018255000

C -0.732142000 1.146217000 -1.407475000

O -0.947057000 2.091279000 2.066311000

O -0.933998000 1.901458000 -2.255641000

O -3.346622000 -0.946196000 0.027546000

Br 2.260570000 0.266297000 -0.014149000

[Tc(CO)3(H2O)2I]

14

TcC3H4O5I

Tc -0.725070000 -0.123787000 0.000866000

O -0.303168000 -1.925583000 1.317745000

H -0.840027000 -2.004337000 2.121575000

O -0.326808000 -1.721870000 -1.573688000

H 0.625577000 -1.697109000 -1.774604000

H 0.619311000 -1.890321000 1.625468000

H -0.469403000 -2.602471000 -1.188671000

C -0.937192000 1.161967000 1.403580000

C -2.624007000 -0.451937000 -0.010147000

C -0.950858000 1.270744000 -1.291576000

O -1.056250000 1.937081000 2.249548000

O -1.078954000 2.103675000 -2.078867000

O -3.763848000 -0.626001000 -0.016485000

I 2.154269000 0.116285000 0.004751000

[Tc(CO)3(H2O)2(NCS)]

16

TcC4NH4SO5

Tc -0.580127000 -0.121277000 -0.002717000

O -0.184391000 -1.942534000 1.279395000

H -0.785226000 -2.091490000 2.025807000

O -0.239257000 -1.720087000 -1.583571000

H 0.673617000 -1.662430000 -1.910468000

H 0.704533000 -1.900852000 1.668152000

H -0.290450000 -2.594225000 -1.162147000

C -0.791158000 1.155384000 1.411290000

C -2.501558000 -0.407437000 -0.021900000

C -0.793305000 1.291531000 -1.280822000

O -0.913854000 1.923716000 2.261994000

O -0.914598000 2.134306000 -2.057615000

O -3.641794000 -0.567348000 -0.032263000

N 1.578961000 -0.019671000 0.015862000

C 2.749817000 0.077910000 0.037250000

S 4.383522000 0.212739000 0.067012000

[Tc(CO)3(H2O)2(NCO)]

16

TcC4NH4O6

Tc -0.290293000 -0.118907000 -0.000315000

O 0.098577000 -1.835957000 1.435761000

H -0.333432000 -1.776593000 2.301624000

O 0.096612000 -1.847753000 -1.422165000

H -0.335251000 -1.796189000 -2.288567000

H 1.052600000 -1.795638000 1.621125000

H 1.050700000 -1.809052000 -1.607591000

C -0.450673000 1.239081000 1.338289000

C -2.213399000 -0.359942000 0.003519000

C -0.454743000 1.228602000 -1.348973000

O -0.526860000 2.058543000 2.146980000

O -0.534181000 2.041745000 -2.163679000

O -3.357716000 -0.503488000 0.006225000

N 1.870228000 -0.151276000 -0.002437000

C 3.022666000 0.121133000 -0.003548000

O 4.204093000 0.368111000 -0.004606000

[Tc(CO)3(H2O)Cl2]-

12

TcC3H2O4Cl2

Tc -0.088432000 0.000289000 -0.020024000

O 1.068856000 -0.002590000 -1.989250000

H 1.663276000 0.763756000 -1.893253000

H 1.661719000 -0.770058000 -1.893082000

C -1.303345000 -1.371200000 -0.588905000

C -1.308756000 1.364127000 -0.595525000

C -0.893590000 0.003121000 1.713158000

O -2.031275000 -2.199799000 -0.933699000

O -1.365507000 0.004905000 2.767239000

O -2.040256000 2.188024000 -0.943796000

Cl 1.686447000 -1.776492000 0.524718000

Cl 1.679801000 1.786981000 0.514119000

[Tc(CO)3(H2O)Br2]-

12

TcC3H2O4Br2

Tc -0.000026000 0.490907000 -0.046556000

O 0.002382000 -0.338284000 -2.186964000

H 0.768797000 -0.939579000 -2.205630000

H -0.765808000 -0.937238000 -2.208314000

C -1.369562000 1.772115000 -0.446919000

C 1.367787000 1.774445000 -0.445261000

C -0.001725000 1.039623000 1.782552000

O -2.191086000 2.546114000 -0.693475000

O -0.002735000 1.362328000 2.891834000

O 2.188246000 2.549814000 -0.691045000

Br -1.904977000 -1.416594000 0.251644000

Br 1.907758000 -1.413283000 0.254386000

[Tc(CO)3(H2O)I2]-

12

TcC3H2O4I2

Tc -0.000058000 0.799547000 -0.071789000

O -0.000360000 0.164974000 -2.278702000

H 0.767448000 -0.424448000 -2.384667000

H -0.767685000 -0.424863000 -2.384484000

C -1.370556000 2.109292000 -0.362909000

C 1.370314000 2.109341000 -0.363251000

C -0.000122000 1.179500000 1.801091000

O -2.183675000 2.911413000 -0.538041000

O -0.000063000 1.397401000 2.935791000

O 2.183324000 2.911544000 -0.538526000

I 2.102123000 -1.229609000 0.162079000

I -2.102113000 -1.229722000 0.162178000

[Tc(CO)3(H2O)(NCS)2]-

16

TcC5N2H2S2O4

Tc -0.001111000 -0.762586000 -0.108514000

O -0.001961000 -0.299563000 -2.349900000

H -0.770004000 0.262215000 -2.543968000

H 0.764461000 0.264174000 -2.545045000

C 1.367494000 -2.120480000 -0.317834000

C -1.373615000 -2.116823000 -0.316610000

C -0.000798000 -1.050607000 1.782142000

O 2.175305000 -2.932927000 -0.448527000

O -0.000571000 -1.206642000 2.925920000

O -2.183664000 -2.927254000 -0.446108000

N -1.476529000 0.832936000 -0.018629000

N 1.479714000 0.827982000 -0.018562000

C 2.244518000 1.706933000 0.113520000

C -2.237676000 1.715436000 0.110752000

S -3.304738000 2.954223000 0.290692000

S 3.316864000 2.940610000 0.297287000

[Tc(CO)3Cl3]-2

10

TcC3O3Cl3

Tc 0.131438000 0.002954000 0.002572000

C 1.208908000 1.091032000 1.144568000

C 1.221000000 -1.524758000 0.372784000

C 1.219017000 0.447606000 -1.506464000

O 1.856070000 1.752735000 1.839951000

O 1.875555000 0.715211000 -2.421242000

O 1.879282000 -2.450031000 0.596292000

Cl -1.436902000 -0.596153000 1.984686000

Cl -1.438393000 2.012954000 -0.494094000

Cl -1.424924000 -1.432856000 -1.504562000

[Tc(CO)3Br3]-2

10

TcC3O3Br3

Tc -0.004184000 0.001665000 0.558894000

C -1.055067000 1.178715000 1.635063000

C -0.507239000 -1.501911000 1.627840000

C 1.542808000 0.312549000 1.639268000

O -1.694136000 1.891926000 2.285193000

O 2.478998000 0.501763000 2.292303000

O -0.810765000 -2.412479000 2.273970000

Br -2.169511000 -0.438105000 -1.065965000

Br 0.716730000 2.100108000 -1.051568000

Br 1.468974000 -1.657764000 -1.056258000

[Tc(CO)3I3]-2

10

TcC3O3I3

Tc 0.004038000 0.003439000 0.829395000

C 0.529943000 -1.490062000 1.900579000

C 1.036048000 1.202007000 1.900067000

C -1.551955000 0.292547000 1.902293000

O 0.844557000 -2.386108000 2.562196000

O -2.484879000 0.466670000 2.564772000

O 1.657469000 1.921644000 2.559964000

I -1.583827000 -1.860397000 -0.853027000

I 2.398301000 -0.445674000 -0.861648000

I -0.821491000 2.301589000 -0.854844000

[Tc(CO)3(NCS)3]-2

16

TcC6N3S3O3

Tc 0.018673000 0.002761000 0.852865000

C -1.527379000 -0.155779000 2.006226000

C 0.966734000 -1.289937000 1.937208000

C 0.706069000 1.439766000 1.952085000

O -2.444414000 -0.261687000 2.698893000

O 1.109784000 2.297108000 2.611120000

O 1.535270000 -2.057415000 2.585051000

N -0.999903000 1.425374000 -0.464281000

N -0.749098000 -1.565928000 -0.471331000

N 1.707725000 0.147904000 -0.535873000

C -1.182824000 -2.428378000 -1.133988000

C 2.630123000 0.221011000 -1.253400000

C -1.533078000 2.215975000 -1.143687000

S -1.792410000 -3.641552000 -2.070913000

S 3.928124000 0.323006000 -2.266599000

S -2.285489000 3.330709000 -2.098900000

*fac*-[Tc(H2O)3(CO)3]+

16

TcC3H6O6

Tc -0.132265000 -0.000785000 -0.002098000

C 0.988092000 -1.055074000 1.146359000

C 0.990175000 -0.466060000 -1.490287000

C 0.986904000 1.523953000 0.338232000

O 1.656063000 -0.745486000 -2.386297000

O 1.648199000 -1.692792000 1.840664000

O 1.650014000 2.441000000 0.546508000

H -2.247213000 1.622805000 -0.684680000

H -1.406005000 1.576396000 -1.980725000

H -2.240169000 -1.418091000 -1.060386000

H -1.383661000 -2.509570000 -0.379518000

H -1.392395000 0.919587000 2.361325000

H -2.248372000 -0.210363000 1.745387000

O -1.688439000 -1.594490000 -0.280056000

O -1.691950000 0.552475000 1.515383000

O -1.700526000 1.034878000 -1.232218000

*fac*-[Tc(DMS)(H2O)2(CO)3]+

22

TcC5H10SO5

Tc -0.484652000 -0.103601000 -0.060393000

C -0.301631000 0.539057000 1.737834000

C -2.422708000 -0.212018000 0.167619000

C -0.668928000 1.707891000 -0.667577000

O -0.185148000 0.918897000 2.819592000

O -3.561526000 -0.256385000 0.302807000

O -0.782783000 2.792698000 -1.039053000

O -0.563832000 -1.121389000 -2.074562000

H 0.198998000 -0.934932000 -2.646006000

O -0.157511000 -2.279229000 0.455998000

H -0.444385000 -2.840441000 -0.283315000

H -0.636446000 -2.612197000 1.230240000

H -1.342968000 -0.937756000 -2.622004000

S 2.012716000 -0.127056000 -0.589151000

C 2.874585000 -1.222610000 0.583231000

H 2.487217000 -2.225493000 0.432641000

H 3.936195000 -1.192241000 0.347877000

H 2.697558000 -0.898805000 1.606128000

C 2.761145000 1.469997000 -0.140270000

H 3.829668000 1.408249000 -0.333563000

H 2.315466000 2.228745000 -0.777741000

H 2.572882000 1.694930000 0.906765000

*fac*-[Tc(CH3CN)(H2O)2(CO)3]+

19

TcC5NH7O5

Tc -0.361211000 -0.090673000 -0.003950000

C -0.585390000 1.209624000 1.392963000

C -0.593539000 1.301888000 -1.307949000

C -2.280290000 -0.394520000 -0.005903000

O -0.725263000 2.129960000 -2.096090000

O -0.716325000 1.986646000 2.231997000

O -3.417061000 -0.563277000 -0.002915000

H 0.189946000 -2.551566000 -1.063238000

H -0.585029000 -1.852896000 -2.196692000

H -0.596365000 -2.124498000 1.941269000

H 0.903199000 -1.796477000 1.805335000

O 0.082661000 -1.880216000 1.293515000

O 0.096329000 -1.700879000 -1.523950000

N 1.806441000 0.062995000 0.011847000

C 2.955350000 0.070159000 0.007131000

C 4.403090000 0.076642000 -0.000737000

H 4.757979000 0.909984000 -0.605921000

H 4.770633000 0.183675000 1.019125000

H 4.764827000 -0.860865000 -0.422103000

*fac*-[Tc(H2O)2(CO)4]+

15

TcC4H4O6

Tc 0.002280000 -0.134134000 -0.000093000

C -0.007595000 1.167776000 1.431284000

C 0.011281000 1.292610000 -1.307762000

C -2.031780000 -0.125613000 -0.015134000

O 0.017315000 2.126712000 -2.094270000

O -0.014036000 1.932055000 2.286519000

O -3.167020000 -0.081869000 -0.020919000

H -0.060369000 -2.641214000 -1.091144000

H -0.578577000 -1.751227000 -2.239872000

H -0.775289000 -2.103964000 1.852423000

H 0.762278000 -2.116633000 1.849551000

O -0.006614000 -1.991644000 1.271458000

O 0.086137000 -1.788645000 -1.534728000

C 2.042711000 -0.130477000 -0.002386000

O 3.177462000 -0.092944000 -0.011495000

*fac*-[Tc(DMS)2(H2O)(CO)3]+

28

TcC7H14S2O4

Tc -0.175019000 0.583168000 -0.108681000

C -0.179132000 0.520462000 1.805116000

C -1.982158000 1.299787000 -0.075109000

C 0.535156000 2.399598000 -0.060249000

O -0.182983000 0.469613000 2.956899000

O -3.045505000 1.734922000 -0.042010000

O 0.937738000 3.474281000 -0.018031000

O -0.023306000 0.465987000 -2.379008000

H -0.673496000 -0.097974000 -2.826276000

H -0.081759000 1.320340000 -2.833698000

S 2.265122000 -0.226309000 -0.386489000

C 2.354123000 -1.855800000 -1.197302000

H 1.865200000 -1.764430000 -2.163540000

H 3.405198000 -2.097780000 -1.338928000

H 1.871230000 -2.625421000 -0.600532000

C 3.007601000 -0.629882000 1.225906000

H 4.019149000 -0.988885000 1.050965000

H 3.038928000 0.290193000 1.803690000

H 2.422973000 -1.383474000 1.748227000

S -1.020473000 -1.820725000 -0.402592000

C -2.839820000 -1.875004000 -0.347838000

H -3.145105000 -2.914970000 -0.439522000

H -3.207008000 -1.447470000 0.581933000

H -3.208206000 -1.310367000 -1.200303000

C -0.651848000 -2.810256000 1.082598000

H -1.105857000 -2.358886000 1.961052000

H -1.042133000 -3.812416000 0.921227000

H 0.427387000 -2.855425000 1.199248000

*fac*-[Tc(CH3CN)2(H2O)(CO)3]+

22

TcC7N2H8O4

Tc 0.533143000 -0.003252000 -0.080973000

C 0.789624000 -0.023844000 1.823349000

C 1.872669000 -1.399920000 -0.272455000

O 0.925162000 -0.040277000 2.966446000

O 2.663170000 -2.226485000 -0.385831000

H 0.794659000 -0.011629000 -2.883877000

H -0.554721000 -0.669028000 -2.551815000

O 0.029001000 0.062129000 -2.293467000

N -1.051964000 1.475713000 0.017744000

N -1.094314000 -1.437008000 -0.006128000

C -1.947550000 2.194123000 0.025652000

C -2.000705000 -2.140265000 0.047217000

C -3.079745000 3.096427000 0.034914000

H -3.985166000 2.537375000 0.268021000

H -2.923849000 3.867191000 0.788024000

H -3.180681000 3.559387000 -0.945885000

C -3.146344000 -3.021968000 0.122575000

H -3.797990000 -2.842402000 -0.731735000

H -2.809501000 -4.057511000 0.114028000

H -3.692206000 -2.822396000 1.044061000

C 1.913560000 1.356299000 -0.252023000

O 2.727418000 2.160932000 -0.355084000

*fac*-[Tc(H2O)(CO)5]+

14

TcC5H2O6

Tc -0.002042000 0.002458000 -0.098164000

C 0.828789000 -1.859969000 -0.135962000

C 0.013358000 -0.012073000 1.849650000

C -1.869846000 -0.822189000 -0.097782000

O 0.021351000 -0.020581000 2.992664000

O 1.296850000 -2.893239000 -0.139261000

O -2.906572000 -1.281243000 -0.079116000

H -0.477339000 -0.692335000 -2.781728000

H 0.790468000 0.175055000 -2.793260000

O -0.073796000 0.083954000 -2.362869000

C 1.864077000 0.827542000 -0.110384000

O 2.901911000 1.284594000 -0.095601000

C -0.830097000 1.872826000 -0.108840000

O -1.290558000 2.908564000 -0.111564000

*fac*-[Tc(DMS)3(CO)3]+

34

TcC9H18S3O3

Tc -0.098568000 -0.090552000 0.533389000

C -1.235190000 1.095068000 1.566193000

C 1.325040000 0.143898000 1.836352000

C -0.790100000 -1.601723000 1.550564000

O -1.913800000 1.780755000 2.193057000

O 2.151521000 0.294893000 2.621995000

O -1.186555000 -2.483201000 2.172401000

S -1.807652000 -0.420997000 -1.368367000

C -2.742533000 1.114711000 -1.655180000

H -2.042411000 1.858725000 -2.027218000

H -3.488581000 0.913582000 -2.420369000

H -3.216951000 1.455915000 -0.738338000

C -3.152833000 -1.513623000 -0.813558000

H -3.881365000 -1.581196000 -1.618340000

H -2.716308000 -2.492560000 -0.632760000

H -3.613057000 -1.127085000 0.092203000

S 0.781449000 1.826731000 -0.944523000

C 2.568643000 2.055879000 -0.670637000

H 2.895425000 2.891082000 -1.285888000

H 2.769633000 2.251969000 0.379475000

H 3.078209000 1.150582000 -0.988065000

C 0.191727000 3.423254000 -0.293583000

H 0.481658000 3.538418000 0.747859000

H 0.624640000 4.213086000 -0.903093000

H -0.890849000 3.441877000 -0.388511000

S 1.179625000 -1.831295000 -0.897836000

C 2.849570000 -2.122575000 -0.235141000

H 3.340840000 -2.854765000 -0.871888000

H 3.424303000 -1.200405000 -0.203017000

H 2.729096000 -2.527969000 0.766212000

C 1.592261000 -1.203647000 -2.558631000

H 2.065319000 -2.013573000 -3.109251000

H 0.658665000 -0.928260000 -3.041594000

H 2.258398000 -0.346421000 -2.506596000

*fac*-[Tc(CH3CN)3(CO)3]+

25

TcC9N3H9O3

Tc -0.650813000 0.002825000 -0.009329000

N 0.721144000 1.090958000 1.290536000

N 0.713425000 0.586113000 -1.606280000

N 0.715214000 -1.669023000 0.289276000

C 1.497345000 1.627022000 1.944844000

C 1.488075000 -2.502630000 0.451098000

C 1.487651000 0.873574000 -2.404248000

C -1.772727000 -1.023229000 -1.219087000

C -1.767789000 -0.537322000 1.487138000

C -1.772203000 1.567146000 -0.286507000

C 2.480480000 2.302337000 2.766971000

H 3.142600000 1.564608000 3.218989000

H 3.063799000 2.982968000 2.147898000

H 1.974869000 2.865833000 3.550120000

C 2.470160000 1.236250000 -3.405461000

H 3.317488000 1.720328000 -2.920941000

H 2.810806000 0.338711000 -3.920207000

H 2.021681000 1.920891000 -4.124081000

C 2.468008000 -3.549588000 0.654415000

H 2.884824000 -3.846812000 -0.307144000

H 3.265914000 -3.177892000 1.296535000

H 1.991138000 -4.407875000 1.125963000

O -2.427585000 -0.855146000 2.372763000

O -2.436738000 2.489887000 -0.452373000

O -2.435431000 -1.633322000 -1.932994000

[Tc(CO)6]+

13

TcC6O6

Tc 0.000184000 0.000186000 0.000428000

C 0.001646000 -0.001616000 2.045392000

C -0.001678000 2.045059000 0.000593000

C 0.001585000 -0.001438000 -2.044334000

C -2.044407000 0.001411000 -0.001638000

C -0.001769000 -2.044581000 0.001525000

C 2.044855000 0.001405000 -0.001026000

O 3.176945000 0.002134000 -0.002254000

O 0.002703000 -0.003101000 3.177474000

O -3.176489000 0.002066000 -0.002533000

O -0.002820000 3.177142000 0.001085000

O 0.002070000 -0.001998000 -3.176417000

O -0.002826000 -3.176671000 0.001705000

[Tc(benzene)2]+

25

TcC12H12

Tc 0.000000000 0.000000000 0.000000000

C -0.976699000 0.662696000 1.955057000

H -1.817429000 0.198473000 2.449916000

C 0.340443000 0.234347000 2.246085000

H 0.504111000 -0.556466000 2.963419000

C 1.439809000 0.817004000 1.571626000

H 2.442614000 0.469910000 1.773834000

C 1.221978000 1.829843000 0.607351000

H 2.058617000 2.255966000 0.073071000

C -0.095223000 2.258756000 0.317185000

H -0.263187000 3.012419000 -0.438092000

C -1.194715000 1.675768000 0.991132000

H -2.201559000 1.984922000 0.750143000

C 0.976700000 -0.662698000 -1.955055000

H 1.817432000 -0.198477000 -2.449914000

C -0.340440000 -0.234345000 -2.246087000

H -0.504106000 0.556468000 -2.963420000

C -1.439807000 -0.817002000 -1.571629000

H -2.442611000 -0.469907000 -1.773839000

C -1.221979000 -1.829841000 -0.607353000

H -2.058619000 -2.255963000 -0.073073000

C 0.095220000 -2.258757000 -0.317182000

H 0.263181000 -3.012419000 0.438096000

C 1.194713000 -1.675771000 -0.991130000

H 2.201556000 -1.984926000 -0.750140000

[Tc(toluene)2]+

31

TcC14H16

Tc 0.000002000 0.000001000 0.000001000

C -1.027546000 -0.789035000 1.907962000

C -1.763495000 -1.224092000 0.773407000

H -1.933675000 -2.281104000 0.624158000

C -2.255565000 -0.298068000 -0.176083000

H -2.795603000 -0.651094000 -1.042592000

C -2.009545000 1.084684000 -0.010401000

H -2.360693000 1.790395000 -0.749069000

C -1.271826000 1.534373000 1.109391000

H -1.056740000 2.586308000 1.229304000

C -0.784283000 0.602839000 2.055883000

H -0.200307000 0.952915000 2.895609000

C -0.554379000 -1.770470000 2.943900000

H -1.326751000 -1.893411000 3.707084000

H 0.350336000 -1.420496000 3.438635000

H -0.360888000 -2.748337000 2.505434000

C 1.027543000 0.789031000 -1.907964000

C 1.763493000 1.224097000 -0.773412000

H 1.933669000 2.281110000 -0.624171000

C 2.255568000 0.298080000 0.176083000

H 2.795606000 0.651112000 1.042590000

C 2.009554000 -1.084673000 0.010406000

H 2.360707000 -1.790380000 0.749076000

C 1.271833000 -1.534372000 -1.109383000

H 1.056752000 -2.586309000 -1.229289000

C 0.784282000 -0.602845000 -2.055879000

H 0.200304000 -0.952927000 -2.895602000

C 0.554371000 1.770460000 -2.943905000

H 1.326742000 1.893401000 -3.707091000

H -0.350344000 1.420480000 -3.438638000

H 0.360877000 2.748328000 -2.505444000

[Tc(tetralin)2]+

45

TcC20H24

Tc 0.000001000 0.000003000 -0.000009000

C 0.980045000 0.986446000 1.800811000

H 0.957074000 0.632870000 2.822719000

C -0.040694000 1.845083000 1.337925000

H -0.840143000 2.143336000 2.001185000

C -0.031254000 2.278862000 -0.007271000

H -0.819267000 2.916081000 -0.382259000

C 1.003621000 1.853282000 -0.869439000

H 1.001109000 2.173150000 -1.902835000

C 2.047499000 1.005913000 -0.410867000

C 2.030414000 0.558228000 0.943127000

C 3.135346000 -0.316513000 1.492556000

H 2.711461000 -1.042259000 2.188229000

H 3.793872000 0.328922000 2.084513000

C 3.959761000 -1.005612000 0.404266000

H 4.835957000 -1.472080000 0.856933000

H 3.375349000 -1.807305000 -0.057253000

C 4.382288000 0.006348000 -0.661304000

H 5.028699000 -0.461515000 -1.404959000

H 4.967782000 0.799817000 -0.187248000

C 3.163579000 0.614748000 -1.364538000

H 2.771909000 -0.089179000 -2.102022000

H 3.458620000 1.505399000 -1.922830000

C -0.980061000 -0.986439000 -1.800823000

H -0.957103000 -0.632863000 -2.822731000

C 0.040688000 -1.845072000 -1.337951000

H 0.840131000 -2.143319000 -2.001221000

C 0.031267000 -2.278854000 0.007244000

H 0.819286000 -2.916070000 0.382221000

C -1.003601000 -1.853281000 0.869425000

H -1.001077000 -2.173150000 1.902820000

C -2.047489000 -1.005915000 0.410866000

C -2.030422000 -0.558228000 -0.943127000

C -3.135366000 0.316507000 -1.492541000

H -2.711495000 1.042253000 -2.188223000

H -3.793896000 -0.328934000 -2.084489000

C -3.959771000 1.005603000 -0.404242000

H -4.835977000 1.472063000 -0.856899000

H -3.375359000 1.807303000 0.057267000

C -4.382278000 -0.006358000 0.661336000

H -5.028679000 0.461504000 1.405000000

H -4.967776000 -0.799828000 0.187290000

C -3.163556000 -0.614753000 1.364553000

H -2.771878000 0.089177000 2.102030000

H -3.458587000 -1.505404000 1.922851000

[Tc(mesitylene)2]+

43

TcC18H24

Tc 0.002084000 -0.003150000 0.000086000

C 1.802145000 1.426048000 0.123740000

C 1.795372000 0.801665000 -1.150543000

H 1.769411000 1.419117000 -2.038967000

C 1.809337000 -0.609867000 -1.291909000

C 1.797971000 -1.401467000 -0.114602000

H 1.774182000 -2.479641000 -0.205594000

C 1.803833000 -0.817961000 1.178577000

C 1.790898000 0.597749000 1.274786000

H 1.760800000 1.057776000 2.254069000

C 1.855023000 2.923327000 0.250382000

H 1.384222000 3.411299000 -0.602286000

H 2.897090000 3.250866000 0.288634000

H 1.367416000 3.261824000 1.163751000

C 1.874458000 -1.246673000 -2.652520000

H 1.406697000 -2.230636000 -2.654239000

H 2.919293000 -1.374042000 -2.947024000

H 1.390949000 -0.625566000 -3.405600000

C 1.864157000 -1.673062000 2.414323000

H 1.372562000 -1.188543000 3.257279000

H 2.907997000 -1.842530000 2.690771000

H 1.402650000 -2.645833000 2.248151000

C -1.800507000 1.416148000 0.194387000

C -1.788421000 0.862334000 -1.111342000

H -1.760440000 1.527439000 -1.964848000

C -1.801166000 -0.539622000 -1.330318000

C -1.792919000 -1.394087000 -0.198042000

H -1.769169000 -2.465857000 -0.346965000

C -1.804982000 -0.882147000 1.125030000

C -1.793246000 0.525718000 1.299075000

H -1.768411000 0.931461000 2.302082000

C -1.857920000 2.904218000 0.402503000

H -1.377829000 3.193195000 1.336685000

H -2.901248000 3.226542000 0.451387000

H -1.382816000 3.439892000 -0.418515000

C -1.864694000 -1.099267000 -2.724687000

H -1.381213000 -0.436170000 -3.441144000

H -2.909451000 -1.210115000 -3.026222000

H -1.396854000 -2.081388000 -2.782319000

C -1.874141000 -1.805708000 2.310060000

H -2.920428000 -1.992161000 2.565855000

H -1.391940000 -1.369761000 3.184206000

H -1.409290000 -2.766836000 2.093293000

**c) Tc(V) complexes**

*trans*-[TcO2(en)2]+ en = ethylenediamine

27

TcC4N4H16O2

Tc 3.567842000 1.122673000 3.758666000

O 4.904593000 0.005304000 4.053078000

O 2.229418000 2.238158000 3.463012000

N 3.466106000 1.570252000 5.920221000

N 2.134252000 -0.413707000 4.444344000

N 3.669666000 0.672856000 1.597139000

N 4.998808000 2.659370000 3.070968000

C 2.829308000 0.428512000 6.637406000

C 1.657827000 -0.077853000 5.817005000

C 4.844350000 1.367425000 0.995871000

C 4.948213000 2.761733000 1.584288000

H 2.902179000 2.408481000 6.039439000

H 4.372553000 1.772741000 6.332324000

H 2.500325000 0.726886000 7.632468000

H 3.582696000 -0.350716000 6.745863000

H 1.200357000 -0.943816000 6.294563000

H 0.900099000 0.698628000 5.718873000

H 2.614810000 -1.310108000 4.456413000

H 1.338356000 -0.522446000 3.822301000

H 2.812250000 1.011373000 1.166797000

H 3.717988000 -0.321793000 1.395886000

H 5.730529000 0.783821000 1.242175000

H 4.756260000 1.414598000 -0.089159000

H 4.068050000 3.349604000 1.326297000

H 5.828183000 3.275942000 1.198266000

H 5.931129000 2.378388000 3.364923000

H 4.831254000 3.572394000 3.484373000

*trans*-[TcO2(CN)4]3-

11

TcC4N4O2

Tc -0.009212000 0.405904000 -0.000001000

O -0.009394000 2.186251000 0.000001000

O -0.009396000 -1.374443000 0.000002000

C -2.185107000 0.405905000 -0.000001000

C 2.166706000 0.405904000 0.000001000

C -0.009186000 0.405905000 2.175910000

C -0.009184000 0.405904000 -2.175914000

N -0.009150000 0.405904000 3.339656000

N -3.348854000 0.405903000 0.000003000

N 3.330452000 0.405904000 0.000002000

N -0.009151000 0.405906000 -3.339659000

*trans*-[TcO2(im)4]+ im = imidazole

39

TcC12N8H16O2

Tc 0.000240000 -0.000504000 0.000218000

O 0.064444000 -0.000667000 1.764519000

O -0.063958000 -0.000764000 -1.764092000

C -2.176083000 2.043388000 -1.006679000

C -2.035445000 2.195430000 1.158304000

N -3.049681000 2.988485000 -0.608706000

H -2.020532000 1.750318000 -2.029275000

C -2.976954000 3.100500000 0.759799000

H -1.678376000 1.965168000 2.146386000

H -3.651212000 3.520202000 -1.219444000

H -3.583204000 3.794287000 1.314288000

C 2.152830000 2.068867000 1.007165000

C 2.009327000 2.219555000 -1.157720000

N 3.014150000 3.025119000 0.608992000

H 2.001336000 1.773815000 2.029799000

C 2.939790000 3.136074000 -0.759528000

H 1.654584000 1.985157000 -2.145664000

H 3.609143000 3.564358000 1.219564000

H 3.537062000 3.837440000 -1.314232000

C 2.173675000 -2.048515000 1.006470000

C 2.039699000 -2.191670000 -1.159541000

N 3.048563000 -2.991937000 0.607286000

H 2.015592000 -1.759072000 2.029747000

C 2.980325000 -3.098038000 -0.761908000

H 1.685420000 -1.957463000 -2.147706000

H 3.648284000 -3.526114000 1.217666000

H 3.588576000 -3.789266000 -1.317402000

C -2.150965000 -2.071719000 -1.006511000

C -2.012739000 -2.216440000 1.159117000

N -3.014512000 -3.025692000 -0.607652000

H -1.996825000 -1.779571000 -2.029594000

C -2.943100000 -3.133216000 0.761283000

H -1.659760000 -1.979846000 2.147174000

H -3.608794000 -3.565865000 -1.218099000

H -3.542335000 -3.832498000 1.316497000

N -1.543939000 1.542605000 0.043930000

N 1.526613000 1.560307000 -0.043245000

N -1.526499000 -1.561061000 0.043934000

N 1.544606000 -1.543594000 -0.044017000

*trans*-[TcO2(py)4]+ py = pyridine

47

TcC20N4H20O2

Tc 0.000955000 0.000896000 0.000113000

O 0.001082000 0.000655000 1.761714000

O 0.000883000 0.001169000 -1.761496000

N 1.579604000 1.544948000 0.000418000

C 2.067955000 2.030883000 1.157353000

C 2.076930000 2.022121000 -1.156338000

C 3.057995000 2.999534000 1.194978000

H 1.640775000 1.620714000 2.060943000

C 3.067760000 2.989987000 -1.193593000

H 1.656960000 1.604873000 -2.060065000

C 3.570936000 3.492124000 0.000780000

H 3.413459000 3.355353000 2.152265000

H 3.431528000 3.337663000 -2.150745000

H 4.344859000 4.248714000 0.000921000

N -1.577754000 -1.543115000 -0.000299000

C -2.064889000 -2.030873000 1.156377000

C -2.076468000 -2.018254000 -1.157292000

C -3.054904000 -2.999576000 1.193462000

H -1.636859000 -1.622038000 2.060162000

C -3.067310000 -2.986079000 -1.195086000

H -1.657359000 -1.599658000 -2.060803000

C -3.569163000 -3.490185000 -0.000992000

H -3.409439000 -3.356875000 2.150540000

H -3.432120000 -3.332167000 -2.152413000

H -4.343231000 -4.246626000 -0.001258000

N -1.543405000 1.579261000 0.000358000

C -2.027390000 2.069912000 -1.156421000

C -2.023557000 2.073268000 1.157298000

C -2.996621000 3.059400000 -1.193692000

H -1.614426000 1.645760000 -2.060166000

C -2.992324000 3.063202000 1.194911000

H -1.607963000 1.651379000 2.060898000

C -3.492107000 3.569091000 0.000698000

H -3.350253000 3.417344000 -2.150865000

H -3.342611000 3.424094000 2.152203000

H -4.249424000 4.342304000 0.000828000

N 1.544798000 -1.577972000 -0.000147000

C 2.022969000 -2.073885000 -1.157097000

C 2.029600000 -2.067858000 1.156612000

C 2.989839000 -3.065672000 -1.194731000

H 1.607119000 -1.652216000 -2.060679000

C 2.996862000 -3.059269000 1.193863000

H 1.618554000 -1.641868000 2.060362000

C 3.489581000 -3.571632000 -0.000531000

H 3.338185000 -3.428431000 -2.152024000

H 3.350764000 -3.416984000 2.151022000

H 4.244954000 -4.346743000 -0.000673000

**Model 2: Optimized structures at TPSS/def2-SVP/IEF-PCM(UFF) level with GAUSSIAN 09 Rev. D.01 program.**

**a) Tc(0) complex**

Tc2(CO)10

22

Tc 0.000000 0.000000 1.581504

Tc 0.000000 0.000000 -1.581504

C -1.853303 -0.743852 -1.445042

C 0.743852 -1.853303 -1.445042

C 1.853303 0.743852 -1.445042

C 0.000000 0.000000 -3.516380

C -0.743852 -1.853303 1.445042

C 1.853303 -0.743852 1.445042

C 0.000000 0.000000 3.516380

C -1.853303 0.743852 1.445042

C -0.743852 1.853303 -1.445042

C 0.743852 1.853303 1.445042

O 0.000000 0.000000 -4.675911

O 1.173435 -2.924073 -1.386632

O -2.924073 -1.173435 -1.386632

O -1.173435 2.924073 -1.386632

O 2.924073 1.173435 -1.386632

O 1.173435 2.924073 1.386632

O 2.924073 -1.173435 1.386632

O 0.000000 0.000000 4.675911

O -1.173435 -2.924073 1.386632

O -2.924073 1.173435 1.386632

**b) Tc(I) complexes**

*fac*-[Tc(ane-S3)(CO)3]+

28

Tc 0.794392 -0.001738 -0.001921

S -0.761554 0.315482 1.917573

S -0.764268 1.502818 -1.233423

S -0.768470 -1.821382 -0.684554

O 2.576096 -1.964631 1.598403

O 2.577529 -0.401901 -2.501171

O 2.570372 2.367390 0.902618

C 1.906594 -1.232438 0.997369

C 1.905280 -0.250391 -1.567949

C 1.904635 1.479562 0.564506

C -1.623526 1.882556 1.437104

H -2.472703 2.016924 2.128018

H -0.877244 2.662842 1.658872

C -2.104503 -0.955976 1.678620

H -2.429802 -1.251435 2.689226

H -2.952073 -0.457326 1.183921

C -1.634769 -2.182214 0.911957

H -2.487403 -2.842827 0.681377

H -0.894190 -2.768990 1.479415

C -2.110251 -0.972183 -1.664903

H -2.436275 -1.697902 -2.427505

H -2.957017 -0.793231 -0.984587

C -1.638954 0.305409 -2.341672

H -2.492425 0.838376 -2.793511

H -0.902782 0.105743 -3.137108

C -2.099302 1.938377 -0.006243

H -2.420085 2.963442 -0.252828

H -2.951370 1.265325 -0.187787

*trans-*TcCl(CO)3(PPh3)2

76

Tc 0.002254 0.048450 -0.168760

C 0.034234 -0.414335 -2.003536

C -0.030977 -1.856646 0.370526

O -0.068238 -2.989245 0.624638

O 0.082376 -0.628746 -3.157010

Cl 0.089572 1.051214 2.147047

P 2.480423 0.010999 -0.009714

C 3.260050 1.668264 0.232569

C 3.213333 2.617485 -0.812123

C 3.836436 2.033174 1.465427

C 3.753457 3.897846 -0.631761

H 2.761203 2.357163 -1.775235

C 4.366276 3.320522 1.644709

H 3.872962 1.312497 2.287866

C 4.329988 4.253253 0.598221

H 3.718682 4.620560 -1.453916

H 4.810043 3.591973 2.608544

H 4.747292 5.255890 0.739752

C 3.211615 -1.022774 1.351327

C 4.544479 -1.479201 1.248073

C 2.458342 -1.357805 2.493954

C 5.108568 -2.256523 2.268914

H 5.144626 -1.234660 0.365718

C 3.028373 -2.137594 3.512837

H 1.436317 -0.977941 2.594179

C 4.351066 -2.590048 3.403087

H 6.142436 -2.605687 2.174305

H 2.431980 -2.389861 4.396332

H 4.792204 -3.200868 4.198188

C 3.352018 -0.702727 -1.487940

C 4.480242 -0.107394 -2.087778

C 2.891020 -1.940885 -1.985478

C 5.120888 -0.730606 -3.171068

H 4.869254 0.842580 -1.710080

C 3.537817 -2.564718 -3.060090

H 2.021983 -2.426490 -1.529736

C 4.652503 -1.957981 -3.660381

H 5.993493 -0.252166 -3.628611

H 3.165995 -3.525489 -3.431595

H 5.154288 -2.441811 -4.505107

C 0.002726 1.966369 -0.713315

O -0.001165 3.075390 -1.041645

P -2.485632 0.001457 -0.030461

C -3.311977 -1.525876 -0.702990

C -4.491559 -2.032065 -0.113987

C -2.782461 -2.186720 -1.830856

C -5.118318 -3.171606 -0.639796

H -4.921958 -1.539200 0.762780

C -3.415149 -3.322466 -2.357864

H -1.875498 -1.817328 -2.312781

C -4.582719 -3.820938 -1.762255

H -6.028953 -3.552612 -0.165142

H -2.987431 -3.819617 -3.234966

H -5.072204 -4.712461 -2.168584

C -3.204212 0.087201 1.675172

C -4.340994 0.861418 1.983186

C -2.629466 -0.715939 2.682708

C -4.888217 0.835186 3.276252

H -4.809059 1.484197 1.215106

C -3.186130 -0.750227 3.967707

H -1.740747 -1.313810 2.463978

C -4.314058 0.029471 4.269745

H -5.769792 1.444962 3.501547

H -2.729377 -1.379623 4.738874

H -4.742606 0.009621 5.277555

C -3.328417 1.377666 -0.936205

C -3.155999 2.700415 -0.471232

C -4.088383 1.152535 -2.100832

C -3.742339 3.773365 -1.155354

H -2.568144 2.892309 0.433335

C -4.664246 2.232467 -2.789011

H -4.234507 0.133785 -2.472920

C -4.494871 3.542452 -2.318512

H -3.606308 4.793238 -0.780234

H -5.251249 2.044099 -3.694355

H -4.947885 4.382635 -2.855483

*trans-*TcCl(CO)3(PMe2Ph)2

48

Tc 0.033655 0.115644 0.077774

C 0.948203 1.777322 0.047138

C -0.052909 0.051139 -1.899322

O -0.108950 0.018738 -3.059464

O 1.517525 2.804502 0.033556

Cl -1.072442 -2.152687 0.160601

P 2.074156 -1.260161 0.052951

C 3.688203 -0.371972 -0.059617

C 4.687826 -0.485225 0.928023

C 3.921575 0.467493 -1.171204

C 5.895476 0.220228 0.802103

H 4.535310 -1.122893 1.803694

C 5.132068 1.161184 -1.299950

H 3.150548 0.585532 -1.941512

C 6.122484 1.040690 -0.311594

H 6.661092 0.123341 1.579488

H 5.299119 1.803702 -2.171146

H 7.066003 1.588224 -0.409066

C 0.040062 0.080050 2.062596

O 0.035283 0.059503 3.222710

P -2.108474 1.304860 0.120735

C -3.662467 0.323758 -0.038056

C -4.634535 0.273143 0.981635

C -3.880004 -0.409903 -1.224569

C -5.805042 -0.483666 0.810967

H -4.492185 0.822787 1.917018

C -5.053795 -1.154898 -1.396161

H -3.129717 -0.402832 -2.022410

C -6.019887 -1.194746 -0.377896

H -6.551100 -0.512293 1.612529

H -5.210358 -1.713540 -2.325216

H -6.934624 -1.782448 -0.510276

C -2.292271 2.559877 -1.230634

H -1.443864 3.262867 -1.177662

H -2.271647 2.056895 -2.211056

H -3.241542 3.111032 -1.121829

C -2.363816 2.343661 1.625170

H -3.304959 2.915350 1.563534

H -2.368733 1.714689 2.529767

H -1.515183 3.044514 1.693154

C 2.230304 -2.371972 1.514383

H 2.335795 -1.780827 2.438336

H 1.286374 -2.939952 1.562328

H 3.084111 -3.062241 1.410445

C 2.153285 -2.453502 -1.357658

H 1.216808 -3.035333 -1.343574

H 2.222510 -1.902220 -2.309334

H 3.025930 -3.119752 -1.253558

*cis-*TcCl(CO)3(PMe2Ph)2

48

Tc 0.019278 -0.555988 0.131282

C 0.397726 -0.267364 1.972993

C -1.298648 -1.914876 0.569766

C 1.369223 -1.945922 -0.018234

O -2.043765 -2.758875 0.859151

O 0.626756 -0.087656 3.108294

O 2.147659 -2.804877 -0.101883

Cl -0.498811 -0.760843 -2.325986

P 1.818802 1.112642 -0.482236

P -1.823963 1.169187 0.153356

C 3.511422 0.460835 -0.126916

C 4.378806 0.042703 -1.156711

C 3.929903 0.321438 1.214959

C 5.640248 -0.492309 -0.850423

H 4.078001 0.125029 -2.205464

C 5.192479 -0.207022 1.516349

H 3.269311 0.619047 2.036520

C 6.052034 -0.615507 0.484106

H 6.301530 -0.812967 -1.662563

H 5.503190 -0.303042 2.562234

H 7.037025 -1.031876 0.720435

C -3.522254 0.442886 0.075237

C -4.497244 0.675401 1.066331

C -3.843874 -0.384216 -1.024240

C -5.772713 0.098155 0.954877

H -4.275650 1.303622 1.934107

C -5.121307 -0.949937 -1.134209

H -3.078825 -0.595897 -1.781601

C -6.089642 -0.710473 -0.145883

H -6.519504 0.285679 1.734072

H -5.358408 -1.587269 -1.993066

H -7.086133 -1.157142 -0.231118

C 1.899406 1.636719 -2.246807

H 1.900187 0.748977 -2.897336

H 0.990913 2.215616 -2.474704

H 2.792045 2.258951 -2.426457

C 1.838827 2.732292 0.419293

H 0.934058 3.305341 0.158345

H 1.841354 2.557496 1.507303

H 2.731226 3.315866 0.138047

C -1.876519 2.273818 1.632088

H -1.997192 1.668282 2.544998

H -0.916883 2.810353 1.702044

H -2.696051 3.008327 1.559823

C -1.855689 2.358000 -1.265114

H -0.988988 3.036625 -1.199569

H -1.785523 1.777159 -2.198841

H -2.785747 2.949708 -1.246653

*trans-*TcBr(CO)3(PPh3)2

76

Tc 0.016074 0.174195 -0.105266

C 0.034314 1.983677 -0.670034

C 0.031954 0.816983 1.771674

O 0.062607 1.286664 2.832693

O 0.033486 3.091701 -1.046422

P -2.470554 0.094121 -0.059727

C -3.222631 -1.139442 -1.214561

C -3.079713 -0.969784 -2.609420

C -3.885716 -2.284747 -0.730399

C -3.607641 -1.916385 -3.498267

H -2.561455 -0.092705 -3.010319

C -4.404162 -3.234884 -1.623837

H -3.997834 -2.438928 0.346715

C -4.270150 -3.052775 -3.007638

H -3.495994 -1.765917 -4.577318

H -4.914474 -4.121268 -1.232027

H -4.677566 -3.794381 -3.702975

C -3.281822 -0.292624 1.568765

C -4.622123 0.096590 1.787848

C -2.594271 -0.979491 2.588432

C -5.255828 -0.192029 3.004161

H -5.173093 0.632929 1.008553

C -3.232448 -1.264339 3.806269

H -1.566597 -1.315743 2.417785

C -4.561132 -0.870242 4.018482

H -6.294471 0.118823 3.160165

H -2.684366 -1.797908 4.590234

H -5.055552 -1.090469 4.970773

C -3.312027 1.699419 -0.471824

C -4.315128 1.833167 -1.452225

C -2.948482 2.831923 0.289420

C -4.928279 3.077306 -1.675632

H -4.632621 0.968023 -2.041146

C -3.568555 4.068451 0.070989

H -2.181333 2.747706 1.066861

C -4.557598 4.196470 -0.917697

H -5.704151 3.164472 -2.443878

H -3.274907 4.935061 0.672747

H -5.038078 5.164828 -1.093391

C 0.088723 -0.380805 -2.014627

O 0.173536 -0.657243 -3.136008

P 2.499327 0.104975 -0.016446

C 3.169682 1.818704 -0.216670

C 3.482745 2.611298 0.906884

C 3.231611 2.400511 -1.501787

C 3.871044 3.950293 0.745390

H 3.425543 2.186148 1.913941

C 3.628706 3.735471 -1.658840

H 2.966743 1.811562 -2.386770

C 3.951594 4.513859 -0.536334

H 4.113776 4.551775 1.627957

H 3.680255 4.169266 -2.663166

H 4.259709 5.557414 -0.660718

C 3.304581 -0.494847 1.546768

C 4.694104 -0.318958 1.735322

C 2.559950 -1.167672 2.533574

C 5.316597 -0.789058 2.898805

H 5.295447 0.191281 0.975630

C 3.188590 -1.640767 3.697124

H 1.492870 -1.352791 2.375811

C 4.564113 -1.449247 3.884594

H 6.393213 -0.640475 3.034760

H 2.596578 -2.164438 4.455328

H 5.052868 -1.817084 4.793215

C 3.415608 -0.890175 -1.291087

C 2.893048 -2.141219 -1.680812

C 4.659278 -0.473451 -1.813162

C 3.598557 -2.953480 -2.581075

H 1.937734 -2.485269 -1.266088

C 5.357664 -1.288216 -2.716540

H 5.087656 0.490818 -1.523162

C 4.829471 -2.528840 -3.103951

H 3.180292 -3.922326 -2.874611

H 6.318784 -0.948713 -3.117600

H 5.376091 -3.162792 -3.810396

Br -0.130006 -2.444245 0.464329

*cis-*TcBr(CO)3(PPh3)2

76

Tc 0.007872 -0.763110 -1.234965

C -0.194666 0.754575 -2.367098

C 1.328091 -1.491738 -2.435840

C -1.296583 -1.785799 -2.228414

O 2.047979 -1.931396 -3.235932

O -0.335143 1.653818 -3.102934

O -2.004645 -2.458050 -2.857481

P -2.084257 0.144693 0.080156

P 2.067481 0.200248 0.045981

C -3.623672 -0.120557 -0.938562

C -4.723735 -0.885471 -0.506286

C -3.682961 0.502957 -2.205013

C -5.853089 -1.033955 -1.329138

H -4.713628 -1.364853 0.476409

C -4.813020 0.357455 -3.019557

H -2.847887 1.115957 -2.558672

C -5.901660 -0.416465 -2.585959

H -6.698944 -1.634070 -0.976838

H -4.841393 0.851043 -3.996851

H -6.783555 -0.533786 -3.224616

C 3.657252 -0.634475 -0.452511

C 4.783179 0.080862 -0.907932

C 3.743017 -2.038758 -0.327604

C 5.967983 -0.596523 -1.239992

H 4.746964 1.169637 -1.003330

C 4.929478 -2.708060 -0.655649

H 2.872580 -2.607208 0.021198

C 6.045527 -1.990505 -1.114993

H 6.832965 -0.025507 -1.594477

H 4.979172 -3.797655 -0.554332

H 6.970834 -2.516281 -1.374097

Br 0.247159 -2.860875 0.370806

C -2.536207 -0.571804 1.724767

C -2.702774 -1.970640 1.838010

C -2.695966 0.231123 2.874133

C -3.047378 -2.545593 3.069767

H -2.562132 -2.612760 0.964430

C -3.030474 -0.351801 4.106119

H -2.560621 1.314882 2.813022

C -3.211071 -1.739415 4.206478

H -3.180111 -3.630395 3.139722

H -3.154000 0.285642 4.988261

H -3.475927 -2.191696 5.168177

C -2.201655 1.973694 0.346093

C -3.453952 2.578195 0.600811

C -1.051854 2.780785 0.287793

C -3.542934 3.961025 0.804330

H -4.361790 1.966816 0.636833

C -1.143534 4.167394 0.491378

H -0.079254 2.330299 0.071757

C -2.387364 4.758813 0.750166

H -4.518535 4.418178 1.001255

H -0.238284 4.780797 0.438942

H -2.460456 5.840829 0.903610

C 2.151372 0.063553 1.887961

C 3.394448 0.057233 2.557511

C 0.965735 -0.011135 2.640880

C 3.441738 -0.008616 3.957070

H 4.327306 0.102602 1.986454

C 1.015614 -0.074358 4.041506

H -0.000091 -0.036111 2.130180

C 2.253059 -0.073316 4.701758

H 4.411537 -0.013347 4.466157

H 0.083141 -0.137404 4.611873

H 2.293003 -0.130563 5.794871

C 2.453671 1.986695 -0.276155

C 2.651631 2.918062 0.763555

C 2.547207 2.427324 -1.615228

C 2.938004 4.260696 0.468300

H 2.583106 2.598512 1.807633

C 2.842095 3.766279 -1.905365

H 2.403630 1.720900 -2.439452

C 3.035758 4.687914 -0.863925

H 3.088251 4.972343 1.287255

H 2.917400 4.089526 -2.948937

H 3.261910 5.735036 -1.091379

*cis*-TcBr(CO)3(PMe2Ph)2

48

Tc -0.049441 0.012616 -0.575014

C -0.411189 1.753153 -1.246257

C 1.299589 -0.297913 -1.939083

C -1.386299 -0.798808 -1.729629

O 2.072174 -0.482342 -2.787186

O -0.633014 2.822524 -1.671627

O -2.157472 -1.288287 -2.447913

P -1.863804 0.324740 1.161892

P 1.777017 0.899432 0.928635

C -3.555679 0.258080 0.418017

C -4.430002 -0.824905 0.644098

C -3.970971 1.301844 -0.438359

C -5.695262 -0.855643 0.035775

H -4.134895 -1.654820 1.293221

C -5.237382 1.270719 -1.037724

H -3.305217 2.146528 -0.646763

C -6.103954 0.191403 -0.802194

H -6.362111 -1.704424 0.221827

H -5.545680 2.091682 -1.693964

H -7.092126 0.166068 -1.273713

C 3.480805 0.507182 0.326825

C 4.363003 1.503809 -0.138909

C 3.900282 -0.841829 0.307460

C 5.642305 1.158588 -0.603691

H 4.065046 2.556383 -0.147222

C 5.180864 -1.179561 -0.151359

H 3.211911 -1.630438 0.633464

C 6.056404 -0.180954 -0.607123

H 6.315794 1.944513 -0.962476

H 5.492863 -2.229590 -0.158098

H 7.055720 -0.446968 -0.968130

C -1.945170 -0.877825 2.554855

H -1.949407 -1.904485 2.157495

H -1.039804 -0.761606 3.171090

H -2.839520 -0.692935 3.173206

C -1.909228 1.955519 2.041973

H -1.019787 2.047630 2.686832

H -1.898124 2.777751 1.308407

H -2.815944 2.028910 2.665190

C 1.812824 2.731996 1.162655

H 1.863992 3.236830 0.184687

H 0.879960 3.042362 1.659580

H 2.671518 3.036006 1.784444

C 1.822497 0.263195 2.665597

H 0.962319 0.664518 3.227289

H 1.747184 -0.835901 2.636270

H 2.757310 0.572257 3.161690

Br 0.476361 -2.399967 0.449417

[Tc(CH3NC)6]+

37

Tc -0.000423 -0.000040 -0.000351

C -1.270460 1.123190 1.137938

C 0.407848 1.632620 -1.156929

C 1.545811 0.492032 1.239532

C -0.408260 -1.632916 1.156177

C -1.546673 -0.491652 -1.240298

C 1.269753 -1.123957 -1.137869

N -2.005115 1.774793 1.796937

N 2.441395 0.776135 1.957730

N -0.645640 -2.578375 1.825785

N 2.005151 -1.775781 -1.795837

N 0.645601 2.577955 -1.826570

N -2.442479 -0.775001 -1.958511

C -2.885074 2.559015 2.588768

H -3.329925 3.359685 1.974471

H -3.691976 1.925101 2.993012

H -2.330842 3.014085 3.426690

C -3.518010 -1.114033 -2.821453

H -3.943801 -0.199737 -3.267606

H -3.158046 -1.774170 -3.628271

H -4.304995 -1.637037 -2.252765

C 0.934129 3.712238 -2.630616

H 1.600436 4.400145 -2.083696

H 1.431035 3.394892 -3.562653

H -0.000211 4.241031 -2.882972

C 2.889076 -2.560075 -2.583160

H 3.934319 -2.307789 -2.337942

H 2.720696 -3.631273 -2.381813

H 2.713036 -2.363186 -3.653947

C 3.517283 1.116619 2.819635

H 3.594940 0.376403 3.633486

H 4.463137 1.128451 2.252558

H 3.346968 2.114977 3.256213

C -0.933673 -3.712980 2.629547

H -0.008919 -4.283209 2.819214

H -1.361973 -3.391046 3.593511

H -1.658584 -4.364306 2.113237

[Tc(tert.BuNC)6]+

91

Tc 0.009308 -0.004405 0.000313

C -1.291348 -0.046568 -1.572135

C 1.115569 -1.486981 -0.863951

C 1.131427 1.399155 -0.968370

C -1.102622 1.472164 0.866916

C -1.116504 -1.406492 0.966579

C 1.309829 0.047394 1.572768

N -2.038408 -0.065307 -2.465901

N 1.772645 2.199622 -1.520600

N -1.741424 2.310886 1.360982

N 2.055552 0.079861 2.466673

N 1.746252 -2.334077 -1.355561

N -1.763909 -2.204464 1.515071

C -2.976324 -0.076807 -3.566833

C -2.580452 -3.188423 2.191078

C 2.516088 -3.396234 -1.964986

C 2.989985 0.126131 3.569770

C 2.571602 3.190575 -2.207464

C -2.534401 3.351346 1.977882

C 3.381740 -2.780031 -3.086673

H 4.083913 -2.036842 -2.673181

H 3.962451 -3.576881 -3.580725

H 2.745872 -2.287765 -3.841428

C 1.527420 -4.433792 -2.542377

H 2.092614 -5.263044 -2.999451

H 0.884468 -4.842484 -1.744962

H 0.888417 -3.973495 -3.314416

C 3.404770 -4.033698 -0.873445

H 4.078973 -3.280776 -0.431946

H 2.784901 -4.469475 -0.072086

H 4.015934 -4.834858 -1.321480

C -2.348513 -4.555350 1.509334

H -2.651653 -4.517401 0.449645

H -1.285071 -4.841971 1.565074

H -2.949018 -5.326231 2.020485

C -2.149536 -3.234035 3.674151

H -2.283463 -2.247577 4.148664

H -2.768734 -3.970955 4.212399

H -1.090909 -3.530416 3.763098

C -4.058007 -2.755050 2.062919

H -4.702246 -3.501678 2.556618

H -4.219498 -1.775990 2.544386

H -4.351005 -2.682148 1.002205

C -2.918546 -1.469036 -4.234018

H -1.905272 -1.674351 -4.618078

H -3.192435 -2.257465 -3.513133

H -3.628358 -1.500145 -5.077439

C -2.559290 1.026348 -4.565072

H -3.254054 1.026887 -5.421537

H -2.590711 2.018465 -4.084451

H -1.538196 0.844654 -4.940317

C -4.385418 0.200995 -2.997175

H -4.670267 -0.577794 -2.270025

H -4.415117 1.183265 -2.496350

H -5.120174 0.201771 -3.819575

C 3.376334 -1.325056 3.933003

H 2.484709 -1.901093 4.232138

H 3.852449 -1.827133 3.074229

H 4.088529 -1.314483 4.774899

C 4.230254 0.926789 3.113111

H 3.948489 1.957288 2.839030

H 4.962919 0.968464 3.936299

H 4.705286 0.444571 2.242374

C 2.294556 0.823103 4.760421

H 2.990099 0.868332 5.615002

H 1.999734 1.851157 4.490929

H 1.395055 0.263624 5.067153

C -3.449453 3.965031 0.894535

H -2.848623 4.394261 0.075433

H -4.125126 3.199920 0.476729

H -4.059117 4.767304 1.342592

C -3.373125 2.710209 3.106102

H -4.039685 1.930749 2.700413

H -2.717453 2.256018 3.867813

H -3.990563 3.485661 3.589613

C -1.569884 4.415143 2.548354

H -0.893882 3.965638 3.294793

H -0.963812 4.862105 1.742594

H -2.153047 5.214311 3.035411

C 1.916478 4.572678 -1.988311

H 0.894856 4.589237 -2.403150

H 1.867853 4.813261 -0.913093

H 2.516081 5.346777 -2.495845

C 2.598133 2.827328 -3.709144

H 3.054568 1.834998 -3.861525

H 1.576174 2.815255 -4.123876

H 3.192610 3.577061 -4.257439

C 3.995662 3.158269 -1.608515

H 3.970942 3.403670 -0.533514

H 4.448483 2.160642 -1.734858

H 4.627338 3.900268 -2.124938

[Tc(CO)3(H2O)2Cl]

14

Tc -0.049201 -0.103482 0.010605

O 0.873073 -1.446228 1.536801

H 0.921606 -2.365311 1.200995

O 0.923420 -1.630432 -1.281460

H 0.561244 -1.757032 -2.180641

H 1.801497 -1.107715 1.480608

H 1.810654 -1.209847 -1.399370

C -0.673656 1.163427 1.281556

C -1.753578 -0.966384 0.035334

C -0.637602 1.043641 -1.384228

O -1.045756 1.943729 2.063502

O -0.984248 1.748174 -2.246067

O -2.793422 -1.494694 0.049839

Cl 2.330890 0.616537 -0.007913

[Tc(CO)3(H2O)2Br]

14

Tc -0.408819 -0.127902 0.012228

O 0.170854 -1.644690 1.546635

H 0.056133 -2.546394 1.180085

O 0.189929 -1.839674 -1.276278

H -0.256503 -1.930963 -2.141142

H 1.149233 -1.519362 1.592263

H 1.138961 -1.662297 -1.476447

C -0.746195 1.250477 1.275728

C -2.257661 -0.612667 0.037374

C -0.731646 1.108663 -1.392742

O -0.944597 2.098342 2.050542

O -0.912243 1.860960 -2.264886

O -3.388511 -0.898101 0.054158

Br 2.199455 0.173294 -0.002403

[Tc(CO)3(H2O)2I]

14

Tc -0.729691 -0.130613 -0.011269

O -0.302431 -1.908175 1.267974

H -0.837562 -2.015559 2.079102

O -0.332612 -1.723352 -1.537347

H 0.633959 -1.676305 -1.718347

H 0.632924 -1.843063 1.565847

H -0.453319 -2.591866 -1.097830

C -0.927118 1.140089 1.386212

C -2.614463 -0.452767 -0.021493

C -0.949271 1.263893 -1.281906

O -1.036525 1.916452 2.248955

O -1.076399 2.117637 -2.065148

O -3.768387 -0.621494 -0.026267

I 2.084465 0.071458 0.001011

[Tc(CO)3(H2O)2(NCS)]

16

Tc -0.582552 -0.115914 -0.010884

O -0.185483 -1.922183 1.235599

H -0.785432 -2.097685 1.987024

O -0.208550 -1.710111 -1.533165

H 0.720109 -1.613412 -1.831724

H 0.714740 -1.854990 1.617932

H -0.210574 -2.554893 -1.033505

C -0.796637 1.138558 1.399439

C -2.490591 -0.409701 -0.041928

C -0.791516 1.295647 -1.263708

O -0.911989 1.903425 2.271434

O -0.910466 2.161820 -2.034444

O -3.643082 -0.580682 -0.062812

N 1.510461 -0.049364 0.006039

C 2.703403 0.035788 0.004911

S 4.322892 0.141932 0.005051

[Tc(CO)3(H2O)2(NCO)]

16

Tc -0.295812 -0.141443 0.000666

O 0.096273 -1.814688 1.423830

H -0.259261 -1.713791 2.328639

O 0.091445 -1.826935 -1.411574

H -0.269180 -1.729333 -2.314827

H 1.073443 -1.727964 1.510556

H 1.068085 -1.743928 -1.505550

C -0.450367 1.210200 1.322778

C -2.206694 -0.364666 0.004257

C -0.451876 1.197612 -1.334194

O -0.528949 2.046449 2.132766

O -0.532498 2.025643 -2.152339

O -3.365583 -0.500827 0.007472

N 1.813290 -0.264548 -0.000211

C 2.975476 0.066124 -0.000379

O 4.141134 0.344515 -0.000247

[Tc(CO)3(H2O)Cl2]-

12

Tc -0.099481 0.000687 -0.061821

O 1.110135 -0.001952 -1.972341

H 1.659452 0.772895 -1.681479

H 1.661479 -0.774208 -1.678977

C -1.312096 -1.364191 -0.597048

C -1.317902 1.357228 -0.605151

C -0.856719 0.003796 1.673421

O -2.061693 -2.198206 -0.928485

O -1.303149 0.008720 2.753657

O -2.075914 2.182748 -0.938894

Cl 1.662076 -1.746664 0.352312

Cl 1.662750 1.750211 0.346507

[Tc(CO)3(H2O)Br2]-

12

Tc -0.000422 0.511754 -0.091430

O 0.002140 -0.373039 -2.172730

H 0.776612 -0.975381 -2.029469

H -0.771242 -0.977015 -2.030375

C -1.364794 1.786518 -0.455465

C 1.362332 1.789116 -0.452861

C -0.001547 1.014508 1.735278

O -2.196129 2.578681 -0.674723

O -0.003796 1.307647 2.866364

O 2.193972 2.580203 -0.674822

Br -1.872344 -1.377718 0.117456

Br 1.874268 -1.374906 0.119027

[Tc(CO)3(H2O)I2]-

12

Tc 0.000011 0.817550 -0.098985

O -0.000374 0.141169 -2.257013

H 0.773602 -0.471182 -2.258490

H -0.774529 -0.470931 -2.258433

C -1.365934 2.115221 -0.366363

C 1.365927 2.115040 -0.367067

C 0.000111 1.168829 1.763584

O -2.190375 2.929324 -0.520560

O 0.000374 1.368099 2.914619

O 2.189660 2.930268 -0.519103

I 2.053650 -1.184494 0.053099

I -2.053545 -1.184524 0.053482

[Tc(CO)3(H2O)(NCS)2]-

16

Tc -0.000977 -0.765102 -0.081925

O 0.000137 -0.177663 -2.262302

H -0.771713 0.425748 -2.324308

H 0.772081 0.425799 -2.322982

C 1.359708 -2.107113 -0.310352

C -1.366984 -2.101733 -0.310116

C -0.001385 -1.089419 1.785441

O 2.180416 -2.924384 -0.450014

O -0.002103 -1.269298 2.938836

O -2.191136 -2.915554 -0.449666

N -1.440445 0.786158 -0.022853

N 1.444778 0.780389 -0.023330

C 2.256714 1.652910 0.027487

C -2.248690 1.662093 0.027948

S -3.355448 2.856680 0.092203

S 3.362736 2.848117 0.092551

[Tc(CO)3Cl3]-2

10

Tc 0.110148 0.000636 0.000539

C 1.177764 1.082502 1.132997

C 1.189814 -1.512909 0.371779

C 1.188268 0.444430 -1.494639

O 1.851395 1.746046 1.829361

O 1.868077 0.717258 -2.412400

O 1.869127 -2.443294 0.599577

Cl -1.391225 -0.588410 1.960875

Cl -1.394668 1.991442 -0.482675

Cl -1.377649 -1.419007 -1.490923

[Tc(CO)3Br3]-2

10

Tc -0.002554 -0.001910 0.543167

C -1.044585 1.171262 1.605282

C -0.504308 -1.491977 1.600982

C 1.529384 0.308091 1.613650

O -1.680920 1.892441 2.275428

O 2.469963 0.495782 2.287477

O -0.812133 -2.405735 2.267606

Br -2.166665 -0.440005 -1.025178

Br 0.704115 2.095580 -1.011968

Br 1.474311 -1.647062 -1.017705

[Tc(CO)3I3]-2

10

Tc 0.001402 0.000082 0.818138

C 0.526276 -1.481963 1.876205

C 1.028812 1.192786 1.874073

C -1.540367 0.292478 1.879925

O 0.842103 -2.383695 2.553190

O -2.479815 0.471339 2.555722

O 1.655244 1.915554 2.549658

I -1.566262 -1.838490 -0.816447

I 2.375706 -0.432815 -0.822375

I -0.814895 2.270381 -0.818342

[Tc(CO)3(NCS)3]-2

16

Tc 0.023549 0.001953 0.861662

C -1.512662 -0.134462 2.005656

C 0.953209 -1.288060 1.938495

C 0.719157 1.424416 1.948390

O -2.443754 -0.218774 2.706282

O 1.140666 2.287286 2.613696

O 1.518513 -2.069263 2.598021

N -0.972330 1.379741 -0.428163

N -0.725078 -1.516466 -0.436623

N 1.663420 0.145272 -0.496910

C -1.152341 -2.364113 -1.153008

C 2.581440 0.214938 -1.249714

C -1.526322 2.150159 -1.145041

S -1.741077 -3.532285 -2.138304

S 3.845848 0.309473 -2.286097

S -2.284331 3.213121 -2.133865

*fac*-[Tc(H2O)3(CO)3]+

16

Tc -0.140450 0.000320 -0.000082

C 0.980698 -1.038707 1.137700

C 0.977020 -0.465945 -1.470284

C 0.972497 1.510484 0.329274

O 1.657934 -0.754823 -2.367711

O 1.656707 -1.674420 1.838692

O 1.647478 2.435870 0.530445

H -2.237610 1.599131 -0.648341

H -1.409001 1.553595 -1.974196

H -2.236010 -1.362001 -1.062757

H -1.402982 -2.488205 -0.366636

H -1.401648 0.916609 2.342102

H -2.236834 -0.243900 1.707616

O -1.678780 -1.554831 -0.279440

O -1.677835 0.530946 1.487756

O -1.682735 1.014259 -1.206542

*fac*-[Tc(DMS)(H2O)2(CO)3]+

22

Tc -0.474148 -0.121622 -0.069353

C -0.251368 0.496748 1.716411

C -2.385310 -0.210292 0.190764

C -0.654230 1.683493 -0.649236

O -0.099527 0.873165 2.806977

O -3.532130 -0.240177 0.367978

O -0.776292 2.782029 -1.013596

O -0.562250 -1.094031 -2.064024

H 0.198270 -0.913830 -2.655007

O -0.157102 -2.271691 0.380429

H -0.420033 -2.809458 -0.396340

H -0.623950 -2.659630 1.146438

H -1.360855 -0.936942 -2.605943

S 2.012848 -0.147470 -0.566179

C 2.847113 -1.218812 0.659903

H 2.376103 -2.208136 0.575841

H 3.913823 -1.272348 0.395302

H 2.709513 -0.813785 1.673542

C 2.739532 1.484620 -0.177031

H 3.826150 1.421590 -0.339397

H 2.296863 2.203826 -0.881393

H 2.510891 1.769063 0.861012

*fac*-[Tc(CH3CN)(H2O)2(CO)3]+

19

Tc -0.332195 -0.123120 -0.005470

C -0.515756 1.172698 1.382001

C -0.509338 1.269873 -1.294341

C -2.249874 -0.362709 -0.016754

O -0.605842 2.117372 -2.083806

O -0.624658 1.957344 2.232877

O -3.402939 -0.493872 -0.021220

H 0.100496 -2.583813 -0.974452

H -0.621441 -1.887350 -2.166661

H -0.689660 -2.156043 1.893167

H 0.842251 -1.894578 1.796184

O 0.019031 -1.908666 1.266692

O 0.054579 -1.741479 -1.475806

N 1.781077 0.005792 0.006370

C 2.943974 0.069062 -0.000166

C 4.393900 0.152214 -0.013410

H 4.706530 1.013481 -0.626741

H 4.765798 0.282503 1.016172

H 4.814050 -0.773002 -0.440902

*fac*-[Tc(H2O)2(CO)4]+

15

Tc -0.000507 -0.143448 -0.001349

C -0.009077 1.149145 1.422307

C 0.011648 1.276612 -1.295847

C -2.014712 -0.108900 -0.027008

O 0.020549 2.126086 -2.082165

O -0.016551 1.920515 2.285639

O -3.160827 -0.031696 -0.045636

H -0.071141 -2.632688 -1.007215

H -0.557126 -1.780925 -2.222908

H -0.774170 -2.118219 1.844668

H 0.778311 -2.173398 1.780248

O -0.015404 -1.977296 1.243081

O 0.080659 -1.787497 -1.481992

C 2.020450 -0.115740 -0.011110

O 3.166083 -0.041763 -0.027280

*fac*-[Tc(DMS)2(H2O)(CO)3]+

28

Tc -0.172896 0.559452 -0.115170

C -0.185244 0.526877 1.786565

C -1.961580 1.267254 -0.094736

C 0.525160 2.357089 -0.073583

O -0.199873 0.507221 2.950298

O -3.033818 1.713542 -0.066689

O 0.927457 3.444811 -0.021549

O -0.005491 0.424059 -2.343763

H -0.665004 -0.119447 -2.819385

H 0.007508 1.280455 -2.814646

S 2.253820 -0.219646 -0.365848

C 2.365010 -1.790314 -1.295533

H 1.865879 -1.609537 -2.258774

H 3.431345 -2.009082 -1.458314

H 1.877793 -2.617144 -0.758037

C 2.987370 -0.679288 1.244605

H 4.030087 -0.985047 1.069765

H 2.962820 0.228482 1.865105

H 2.419311 -1.486986 1.729225

S -1.005007 -1.839273 -0.346144

C -2.834828 -1.877211 -0.354449

H -3.148734 -2.927430 -0.455426

H -3.234260 -1.434387 0.570086

H -3.163431 -1.303089 -1.232910

C -0.670782 -2.789105 1.181569

H -1.128572 -2.295629 2.051143

H -1.078567 -3.801657 1.042472

H 0.420525 -2.842094 1.300876

*fac*-[Tc(CH3CN)2(H2O)(CO)3]+

22

Tc 0.466496 -0.004852 -0.090421

C 0.718049 0.015515 1.800746

C 1.806649 -1.391330 -0.244431

O 0.861150 0.022706 2.953834

O 2.610294 -2.223776 -0.326588

H 0.751534 -0.029680 -2.876158

H -0.585642 -0.739358 -2.541762

O -0.014574 0.007256 -2.270375

N -1.072172 1.454465 -0.010665

N -1.103041 -1.424913 0.008479

C -1.932164 2.238136 0.019166

C -1.983673 -2.186053 0.046484

C -3.006759 3.215604 0.059948

H -3.955975 2.711632 0.305507

H -2.786522 3.975102 0.828022

H -3.097342 3.706577 -0.923005

C -3.082607 -3.135027 0.094431

H -3.739503 -2.981325 -0.777500

H -2.685499 -4.163279 0.077007

H -3.662339 -2.981695 1.019574

C 1.830971 1.354935 -0.277469

O 2.646339 2.172953 -0.382065

*fac*-[Tc(H2O)(CO)5]+

14

Tc 0.000746 -0.001156 -0.108724

C 0.822139 -1.849671 -0.143594

C 0.013019 -0.012206 1.828720

C -1.853395 -0.812896 -0.090534

O 0.021662 -0.022869 2.981838

O 1.289663 -2.895672 -0.147314

O -2.903537 -1.268913 -0.048426

H -0.482294 -0.694760 -2.790450

H 0.788040 0.201030 -2.797544

O -0.062593 0.062966 -2.335795

C 1.849881 0.822892 -0.103963

O 2.894394 1.292459 -0.069066

C -0.822485 1.853166 -0.124186

O -1.288686 2.898994 -0.123178

*fac*-[Tc(DMS)3(CO)3]+

34

Tc -0.084472 -0.098059 0.516345

C -1.225949 1.055691 1.547604

C 1.338399 0.138771 1.791643

C -0.740412 -1.602977 1.526492

O -1.922969 1.730147 2.187702

O 2.182136 0.285638 2.576545

O -1.121155 -2.491949 2.169407

S -1.788688 -0.470947 -1.348411

C -2.668746 1.078698 -1.760267

H -1.926122 1.758424 -2.203290

H -3.438282 0.837385 -2.509322

H -3.122289 1.519513 -0.860208

C -3.176750 -1.477141 -0.709368

H -3.915151 -1.582138 -1.518726

H -2.762296 -2.462346 -0.451803

H -3.624907 -0.999745 0.174741

S 0.765878 1.840925 -0.918386

C 2.558695 2.106027 -0.650126

H 2.860620 2.972551 -1.257869

H 2.768408 2.280506 0.415415

H 3.085047 1.207539 -1.000783

C 0.136725 3.429707 -0.256855

H 0.420360 3.544262 0.799812

H 0.565202 4.237906 -0.868972

H -0.957169 3.424644 -0.364273

S 1.167463 -1.806684 -0.925531

C 2.817075 -2.193277 -0.235009

H 3.298987 -2.925622 -0.900482

H 3.432465 -1.286833 -0.137637

H 2.642191 -2.645437 0.752316

C 1.605499 -1.157176 -2.579011

H 2.051396 -1.983597 -3.153174

H 0.661736 -0.841577 -3.048279

H 2.306344 -0.312252 -2.512924

*fac*-[Tc(CH3CN)3(CO)3]+

25

Tc -0.557726 0.000828 -0.000087

N 0.756326 1.074587 1.277706

N 0.757099 0.568488 -1.568750

N 0.754308 -1.643845 0.293069

C 1.495220 1.653234 1.965804

C 1.491067 -2.530644 0.451351

C 1.496013 0.873548 -2.414464

C -1.668915 -1.018672 -1.214169

C -1.671337 -0.538717 1.489178

C -1.668284 1.562326 -0.277564

C 2.416177 2.377144 2.826446

H 3.098511 1.665466 3.319737

H 3.004363 3.088490 2.223638

H 1.848898 2.930126 3.593099

C 2.416391 1.254793 -3.473005

H 3.291931 1.763320 -3.036897

H 2.749697 0.354701 -4.015328

H 1.910135 1.937424 -4.175233

C 2.408049 -3.641008 0.649150

H 2.815679 -3.962137 -0.323500

H 3.235624 -3.325138 1.305339

H 1.872845 -4.483869 1.116664

O -2.336743 -0.862245 2.381871

O -2.331683 2.498626 -0.443764

O -2.332311 -1.630210 -1.942398

[Tc(CO)6]+

13

Tc 0.000000 0.000000 0.000000

C 0.000000 0.000000 2.030903

C 0.000000 2.030903 0.000000

C 0.000000 0.000000 -2.030903

C -2.030903 0.000000 0.000000

C 0.000000 -2.030903 0.000000

C 2.030903 0.000000 0.000000

O 3.173630 0.000000 0.000000

O 0.000000 0.000000 3.173630

O -3.173630 0.000000 0.000000

O 0.000000 3.173630 0.000000

O 0.000000 0.000000 -3.173630

O 0.000000 -3.173630 0.000000

[Tc(benzene)2]+

25

Tc 0.000000 0.000000 0.000000

C -0.990277 0.612163 1.914690

H -1.842244 0.131097 2.404952

C 0.339343 0.181070 2.209907

H 0.505310 -0.630803 2.924954

C 1.448768 0.770598 1.530468

H 2.463619 0.408976 1.724057

C 1.229182 1.792724 0.557231

H 2.075863 2.214754 0.006853

C -0.100151 2.224407 0.262259

H -0.270914 2.977167 -0.513600

C -1.209851 1.634224 0.941079

H -2.230171 1.936949 0.686318

C 0.990277 -0.612163 -1.914690

H 1.842244 -0.131097 -2.404952

C -0.339343 -0.181070 -2.209907

H -0.505310 0.630803 -2.924954

C -1.448768 -0.770598 -1.530468

H -2.463619 -0.408976 -1.724057

C -1.229182 -1.792724 -0.557231

H -2.075863 -2.214754 -0.006853

C 0.100151 -2.224407 -0.262259

H 0.270914 -2.977167 0.513600

C 1.209851 -1.634224 -0.941079

H 2.230171 -1.936949 -0.686318

[Tc(toluene)2]+

31

Tc 0.000000 0.000000 0.000000

C -0.988909 -0.787837 1.878206

C -1.729592 -1.225462 0.729914

H -1.896823 -2.296636 0.574773

C -2.210698 -0.292980 -0.237678

H -2.739268 -0.654224 -1.125555

C -1.953512 1.101736 -0.076551

H -2.282296 1.814072 -0.839482

C -1.218448 1.555551 1.059562

H -0.983897 2.618816 1.171720

C -0.739041 0.617674 2.023189

H -0.140154 0.972761 2.868584

C -0.499702 -1.776080 2.910308

H -1.279100 -1.911731 3.683760

H 0.414156 -1.412128 3.407137

H -0.297036 -2.759198 2.455263

C 0.988909 0.787837 -1.878206

C 1.729592 1.225462 -0.729914

H 1.896823 2.296636 -0.574773

C 2.210698 0.292980 0.237678

H 2.739268 0.654224 1.125555

C 1.953512 -1.101736 0.076551

H 2.282296 -1.814072 0.839482

C 1.218448 -1.555551 -1.059562

H 0.983897 -2.618816 -1.171720

C 0.739041 -0.617674 -2.023189

H 0.140154 -0.972761 -2.868584

C 0.499702 1.776080 -2.910308

H 1.279100 1.911731 -3.683760

H -0.414156 1.412128 -3.407137

H 0.297036 2.759198 -2.455263

[Tc(tetralin)2]+

45

Tc -0.000002 0.000002 -0.000005

C 0.913367 0.950092 1.802945

H 0.882031 0.582336 2.833530

C -0.126729 1.799301 1.327366

H -0.952058 2.077340 1.989846

C -0.118081 2.234996 -0.030644

H -0.933549 2.852126 -0.417711

C 0.938330 1.824200 -0.894327

H 0.929377 2.134376 -1.944342

C 2.004983 0.991066 -0.422767

C 1.985472 0.535623 0.944400

C 3.098409 -0.339657 1.492010

H 2.675205 -1.068669 2.204482

H 3.766357 0.318947 2.082231

C 3.917580 -1.035417 0.396172

H 4.800486 -1.516873 0.850536

H 3.317922 -1.840759 -0.070080

C 4.346539 -0.019930 -0.671393

H 5.000224 -0.492319 -1.424570

H 4.941905 0.779424 -0.190032

C 3.128795 0.600217 -1.376552

H 2.723942 -0.102825 -2.125892

H 3.430144 1.503037 -1.937365

C -0.913376 -0.950102 -1.802948

H -0.882048 -0.582353 -2.833537

C 0.126726 -1.799302 -1.327370

H 0.952053 -2.077341 -1.989853

C 0.118087 -2.234989 0.030643

H 0.933561 -2.852113 0.417708

C -0.938320 -1.824193 0.894329

H -0.929359 -2.134361 1.944346

C -2.004980 -0.991067 0.422770

C -1.985478 -0.535631 -0.944399

C -3.098417 0.339648 -1.492006

H -2.675216 1.068656 -2.204483

H -3.766373 -0.318957 -2.082219

C -3.917577 1.035415 -0.396163

H -4.800483 1.516875 -0.850522

H -3.317909 1.840754 0.070082

C -4.346534 0.019932 0.671406

H -5.000212 0.492325 1.424586

H -4.941906 -0.779419 0.190051

C -3.128789 -0.600219 1.376559

H -2.723931 0.102819 2.125901

H -3.430137 -1.503041 1.937369

[Tc(mesitylene)2]+

43

Tc -0.000054 0.000126 -0.000423

C 1.740743 1.440388 0.126897

C 1.729957 0.810941 -1.159214

H 1.696123 1.436745 -2.057008

C 1.744979 -0.612684 -1.305490

C 1.726954 -1.411841 -0.117863

H 1.690147 -2.501999 -0.211671

C 1.737609 -0.826381 1.188755

C 1.724793 0.601899 1.286949

H 1.687117 1.065893 2.277601

C 1.805332 2.942040 0.252998

H 1.327119 3.438810 -0.605578

H 2.864085 3.258849 0.277878

H 1.328998 3.291215 1.182369

C 1.813120 -1.253460 -2.669353

H 1.334296 -2.245149 -2.672358

H 2.872372 -1.389820 -2.954422

H 1.338458 -0.622306 -3.436457

C 1.795950 -1.687417 2.426248

H 1.308658 -1.196743 3.283525

H 2.853040 -1.863973 2.696927

H 1.325074 -2.668374 2.257898

C -1.741784 1.431577 0.195970

C -1.725866 0.870421 -1.121221

H -1.688486 1.541928 -1.985113

C -1.739729 -0.544255 -1.341734

C -1.725808 -1.404347 -0.198070

H -1.687882 -2.488112 -0.348732

C -1.741913 -0.888094 1.137378

C -1.730160 0.532865 1.310421

H -1.696730 0.944081 2.324282

C -1.808188 2.924227 0.404760

H -1.335502 3.221576 1.353980

H -2.867369 3.238100 0.444010

H -1.327881 3.469394 -0.422418

C -1.800591 -1.110180 -2.739086

H -1.321575 -0.437965 -3.468008

H -2.858171 -1.229914 -3.037448

H -1.322406 -2.100529 -2.794196

C -1.805244 -1.815663 2.324921

H -2.863548 -2.010323 2.578070

H -1.325125 -1.373131 3.211652

H -1.329449 -2.783887 2.103801

**c) Tc(V) complexes**

*trans*-[TcO2(en)2]+ en = ethylenediamine

27

Tc 0.000036 -0.000378 0.000258

O -0.000882 -0.001352 -1.755833

O 0.000551 0.000287 1.756478

N 1.686236 1.398636 0.005994

N 1.687121 -1.398485 -0.006021

N -1.687188 -1.398442 0.007769

N -1.686337 1.398731 -0.005808

C 2.949102 0.680047 -0.346457

C 2.950105 -0.678554 0.344389

C -2.949208 -0.679049 -0.346384

C -2.949839 0.679923 0.343733

H 1.755756 1.790137 0.954643

H 1.549623 2.200464 -0.621462

H 3.837166 1.266377 -0.055530

H 2.963902 0.555631 -1.441529

H 3.838056 -1.264438 0.052300

H 2.966387 -0.553831 1.439358

H 1.756680 -1.791047 -0.954323

H 1.552482 -2.199936 0.622496

H -1.757454 -1.787874 0.957202

H -1.551565 -2.201916 -0.618082

H -2.962692 -0.555242 -1.441517

H -3.838018 -1.264625 -0.055989

H -2.967390 0.555748 1.438825

H -3.837351 1.266067 0.050390

H -1.755225 1.793959 -0.953075

H -1.549033 2.198032 0.624828

*trans*-[TcO2(CN)4]3-

11

Tc -0.000005 0.000000 0.000000

O 0.000016 0.000000 -1.774195

O 0.000017 0.000000 1.774195

C 2.155310 -0.003126 0.000000

C -2.155303 0.003126 0.000000

C -0.003133 -2.155306 0.000000

C 0.003120 2.155307 0.000000

N -0.004611 -3.336952 0.000000

N 3.336956 -0.004605 0.000000

N -3.336949 0.004604 0.000000

N 0.004599 3.336953 0.000000

*trans*-[TcO2(im)4]+ im = imidazole

39

Tc 0.000026 0.000353 -0.000067

O 0.063665 -0.000121 1.756009

O -0.063538 -0.000574 -1.756145

C -2.190273 1.979533 -1.020191

C -2.008105 2.177164 1.150210

N -3.078175 2.922825 -0.619965

H -2.044489 1.660754 -2.050576

C -2.981747 3.066116 0.748629

H -1.618540 1.965504 2.144265

H -3.708136 3.436359 -1.235300

H -3.598162 3.770341 1.303486

C 2.168708 2.003175 1.020150

C 1.981280 2.202038 -1.149691

N 3.044131 2.958241 0.620359

H 2.028262 1.680866 2.050178

C 2.944209 3.102481 -0.747886

H 1.593192 1.987004 -2.143599

H 3.668492 3.478537 1.235720

H 3.551194 3.815118 -1.302399

C 2.181034 -1.989706 1.019891

C 2.016199 -2.166486 -1.153709

N 3.071374 -2.929936 0.617819

H 2.027486 -1.680566 2.052090

C 2.985755 -3.060183 -0.752768

H 1.634234 -1.945411 -2.148672

H 3.696163 -3.449694 1.233217

H 3.606096 -3.759585 -1.309350

C -2.157810 -2.014795 -1.020115

C -1.990732 -2.189766 1.153465

N -3.036791 -2.965667 -0.618063

H -2.008123 -1.703648 -2.052278

C -2.949492 -3.095026 0.752502

H -1.611310 -1.964223 2.148400

H -3.655428 -3.492750 -1.233446

H -3.561356 -3.801871 1.309065

N -1.525645 1.508429 0.037423

N 1.508351 1.525819 -0.037337

N -1.507986 -1.525162 0.038321

N 1.525333 -1.507922 -0.038522

*trans*-[TcO2(py)4]+ py = pyridine

47

Tc -0.000836 -0.000911 -0.000112

O -0.000751 -0.000786 1.754626

O -0.001477 -0.001293 -1.754772

N 1.549114 1.509284 0.000055

C 2.043814 1.993480 1.167073

C 2.044272 1.993618 -1.166824

C 3.040783 2.970140 1.203958

H 1.608755 1.566616 2.075339

C 3.041400 2.970110 -1.203120

H 1.609292 1.567310 -2.075385

C 3.553502 3.472494 0.000541

H 3.404274 3.326294 2.171812

H 3.405559 3.326069 -2.170810

H 4.335057 4.238515 0.000766

N -1.550897 -1.510913 0.000427

C -2.043828 -1.996762 1.167580

C -2.048179 -1.993498 -1.166339

C -3.040965 -2.973133 1.204689

H -1.607165 -1.571362 2.075765

C -3.045155 -2.970072 -1.202401

H -1.615074 -1.565439 -2.074990

C -3.555476 -3.473973 0.001410

H -3.403209 -3.330211 2.172689

H -3.410599 -3.324942 -2.170006

H -4.337096 -4.239912 0.001807

N -1.511179 1.548652 -0.000166

C -1.994325 2.044759 -1.167085

C -1.996836 2.042268 1.166824

C -2.970926 3.041772 -1.203694

H -1.566908 1.610554 -2.075520

C -2.973501 3.039158 1.203372

H -1.570927 1.606523 2.075194

C -3.474657 3.552828 -0.000166

H -3.325863 3.406563 -2.171517

H -3.330633 3.401799 2.171202

H -4.240871 4.334186 -0.000167

N 1.511269 -1.548821 -0.000476

C 1.994462 -2.044479 -1.167607

C 1.999969 -2.039988 1.166257

C 2.973979 -3.038545 -1.204608

H 1.564814 -1.612145 -2.075857

C 2.979851 -3.033777 1.202421

H 1.573975 -1.604815 2.074875

C 3.480919 -3.547014 -0.001283

H 3.328658 -3.403160 -2.172596

H 3.339417 -3.394355 2.170121

H 4.249531 -4.326011 -0.001628

**Explicit Solvent: Optimized structures with 14 water explicit molecules at TPSS/def2-SVP/IEF-PCM(UFF) level with GAUSSIAN 09 Rev. D.01 program**

***trans*-[TcO2(en)2]+ en = ethylenediamine**

**Configuration 01**

69

Tc 0.309376 -0.311663 -0.178367

O -1.413571 -0.212840 0.093759

O 2.044229 -0.274392 -0.545366

N -0.120770 0.440388 -2.202746

N 0.013230 -2.194022 -1.247270

N 0.593903 -1.033361 1.849213

N 0.515458 1.573692 0.885881

C -0.689448 -0.661846 -3.031787

C 0.050498 -1.957354 -2.717616

C 0.576597 0.104925 2.818260

C 1.215512 1.330664 2.173440

H 0.748799 0.789421 -2.623839

H -0.794449 1.232448 -2.169529

H -0.631536 -0.424498 -4.108513

H -1.754169 -0.756553 -2.760596

H -0.400126 -2.802132 -3.269613

H 1.106592 -1.875447 -3.028247

H -0.941645 -2.535964 -0.966114

H 0.680505 -2.948844 -1.006275

H 1.487683 -1.569453 1.971020

H -0.197970 -1.669296 2.073266

H -0.476442 0.324311 3.063111

H 1.094467 -0.169828 3.754067

H 2.283826 1.148571 1.966301

H 1.140502 2.207728 2.842022

H -0.440897 1.945094 1.099137

H 0.973440 2.319258 0.324943

O -3.639269 1.036060 0.061188

H -2.765646 0.508320 0.071274

H -4.246929 0.387661 -0.382940

O 3.930874 -2.288971 -0.235602

H 3.356603 -1.510424 -0.449426

H 3.379265 -3.054112 -0.537696

O 4.239009 1.273442 -0.830197

H 4.323468 1.402528 -1.793297

H 3.417751 0.706970 -0.737736

O 2.091376 -4.291225 -0.813472

H 2.182331 -4.894602 -1.576019

H 1.983643 -4.887134 -0.046976

O 1.427890 3.841934 -0.736008

H 1.590358 3.599046 -1.666266

H 2.355982 3.899895 -0.327741

O -2.558711 -3.120645 -0.344592

H -3.245026 -2.472426 -0.626854

H -2.403668 -2.882525 0.609082

O -2.002042 -2.323700 2.262008

H -2.596700 -1.526131 2.416303

H -2.223814 -2.940023 2.984551

O 3.100362 -2.349780 2.321511

H 3.504480 -2.348338 1.398806

H 3.630592 -1.686221 2.800972

O -4.708307 -1.231395 -1.076666

H -5.527710 -1.608288 -0.700569

H -4.872862 -1.227497 -2.039974

O -1.969909 2.913752 1.602049

H -1.731670 3.625380 0.932910

H -2.722062 2.452429 1.175609

O 3.822583 3.651819 0.328574

H 4.484097 4.262022 -0.047463

H 4.042451 2.760319 -0.089110

O -3.643319 -0.196912 2.634141

H -3.753443 0.297893 1.780942

H -3.281599 0.473045 3.244146

O -1.243719 4.563312 -0.418116

H -0.265465 4.421848 -0.497095

H -1.617776 3.911334 -1.065770

O -2.276523 2.446007 -1.906203

H -2.890585 2.001451 -1.253257

H -2.827126 2.617320 -2.693126

**Configuration 02**

69

Tc -0.037466 -0.424616 0.259034

O 1.523196 0.120982 -0.393682

O -1.520917 -0.988939 0.986909

N 0.856111 -0.509830 2.275141

N 0.746974 -2.454448 0.260342

N -0.863784 -0.412235 -1.735008

N -0.787444 1.633990 0.150675

C 1.164081 -1.932994 2.612586

C 1.719449 -2.630778 1.373851

C -0.851708 0.982561 -2.244712

C -1.450668 1.888400 -1.172140

H 0.213916 -0.127638 2.979424

H 1.734558 0.059896 2.358533

H 0.227585 -2.422182 2.930439

H 1.883090 -1.993371 3.448620

H 2.674052 -2.170910 1.067702

H 1.903335 -3.700254 1.579451

H 1.151680 -2.682514 -0.663136

H -0.063138 -3.089187 0.348005

H -1.838109 -0.782997 -1.692997

H -0.346996 -1.078615 -2.342493

H 0.197248 1.261073 -2.439842

H -1.417747 1.072934 -3.189615

H -2.526203 1.677075 -1.050317

H -1.339487 2.947928 -1.460052

H -0.012930 2.315989 0.278322

H -1.485790 1.841947 0.892199

O -3.816095 -0.472920 2.267031

H -2.948567 -0.807616 1.901976

H -3.645420 0.509456 2.289203

O 3.287006 2.020024 0.243290

H 2.684776 2.816537 0.229498

H 2.669075 1.289493 -0.062511

O 3.537689 -0.963594 -1.959897

H 4.054870 -1.369994 -1.214252

H 2.778050 -0.554503 -1.468009

O -5.098365 -0.602456 0.023917

H -4.656777 -0.609550 0.961542

H -5.975357 -1.015035 0.139202

O -3.399378 -1.840131 -1.634387

H -3.853195 -1.920703 -2.493779

H -4.079558 -1.432183 -1.011966

O -3.186410 2.140852 1.782066

H -3.307650 2.893960 2.389255

H -3.875526 2.266208 1.054860

O 0.359295 -2.874845 -2.565124

H -0.411513 -3.355540 -2.144535

H 0.538057 -3.349403 -3.396445

O -1.647822 -3.801395 -1.017170

H -2.395398 -3.158638 -1.194506

H -2.040606 -4.686929 -1.123469

O 5.140697 -1.340497 0.257927

H 5.383377 -0.439341 -0.115493

H 5.925901 -1.886455 0.066352

O -5.039488 2.101485 -0.128478

H -5.146083 1.108682 -0.205531

H -4.824276 2.403871 -1.029489

O 3.270370 0.965061 2.720388

H 3.367663 1.435085 1.838854

H 2.997461 1.676977 3.328823

O 1.259711 3.785094 0.294362

H 1.149280 4.366611 1.069417

H 0.939092 4.326147 -0.487578

O 0.201453 5.045081 -1.827712

H 0.798311 5.100761 -2.598575

H -0.057704 5.972641 -1.666777

O 5.373178 0.951788 -1.163498

H 4.756931 0.404345 -1.721586

H 4.727873 1.534253 -0.680270

**Configuration 03**

69

Tc -0.518641 -0.495138 -0.008869

O 0.912258 0.384835 0.458576

O -1.980505 -1.434339 -0.414543

N 0.515590 -1.509901 -1.643295

N -0.880874 0.889594 -1.646316

N -1.658974 0.451471 1.605737

N -0.127013 -1.871467 1.644436

C 0.687956 -0.584110 -2.793756

C -0.597959 0.223386 -2.946723

C -1.493125 -0.287117 2.892646

C -1.242498 -1.768899 2.621489

H -0.115938 -2.290310 -1.925695

H 1.413816 -1.959523 -1.362183

H 0.923202 -1.134577 -3.722495

H 1.532104 0.092122 -2.573417

H -0.511250 0.961343 -3.764319

H -1.439057 -0.452000 -3.179443

H -0.221816 1.689496 -1.534597

H -1.828768 1.318698 -1.630302

H -2.661748 0.486271 1.337861

H -1.393398 1.454838 1.764987

H -0.623644 0.143416 3.420161

H -2.375849 -0.153378 3.542602

H -2.130176 -2.235900 2.163787

H -1.010857 -2.305634 3.559194

H 0.739059 -1.526485 2.079257

H 0.084073 -2.857830 1.359201

O -1.575101 -3.496188 -2.111022

H -2.035310 -3.295567 -2.947450

H -1.936199 -2.818976 -1.477226

O 2.566313 1.923130 1.931998

H 2.922627 2.501449 1.211724

H 1.920837 1.358377 1.421875

O -4.634483 -1.524975 -0.230232

H -4.839316 -2.140062 0.499036

H -3.634893 -1.587567 -0.324585

O 4.486457 -1.237485 0.183476

H 4.488466 -0.460201 -0.422992

H 4.358455 -0.837614 1.100117

O -3.278785 2.446126 -1.170427

H -3.814004 1.940361 -0.484131

H -3.913135 2.691115 -1.868593

O 0.840731 -4.380815 0.712891

H 1.230992 -4.843085 1.477425

H 1.623438 -3.934282 0.279151

O 2.753460 -2.990620 -0.621552

H 3.438206 -2.316785 -0.258956

H 3.232967 -3.497233 -1.302744

O 3.222927 3.182690 -0.457593

H 3.759435 3.993815 -0.540239

H 3.768131 2.461622 -0.885443

O -1.462166 4.282661 -0.160780

H -0.648658 4.034807 -0.673163

H -2.167288 3.691447 -0.536393

O 4.162399 -0.093850 2.583280

H 3.603806 0.725212 2.369443

H 3.564967 -0.640338 3.127110

O -0.983183 3.156972 2.210680

H -1.721465 3.443617 2.779624

H -1.164116 3.632270 1.336012

O 0.743915 3.314283 -1.542514

H 1.666169 3.295951 -1.148401

H 0.867281 3.657306 -2.447259

O 4.642098 1.096704 -1.491830

H 5.601516 1.287331 -1.497541

H 4.432385 0.914698 -2.429604

O -4.413286 0.921811 0.681177

H -4.647078 -0.007661 0.342928

H -5.128139 1.185429 1.288493

**Configuration 04**

69

Tc 0.256166 -0.237473 -0.171139

O 0.866937 0.983548 0.970466

O -0.373064 -1.407020 -1.319068

N -1.332570 -0.767283 1.228321

N 1.222664 -1.828661 0.951679

N 1.829292 0.259952 -1.599484

N -0.731428 1.333868 -1.341303

C -0.854346 -1.761946 2.237938

C 0.174470 -2.677971 1.582579

C 1.516465 1.541326 -2.288049

C 0.025088 1.561701 -2.609251

H -2.143717 -1.185981 0.718002

H -1.713119 0.072513 1.708185

H -1.710621 -2.346407 2.620116

H -0.390430 -1.211998 3.074993

H 0.614880 -3.371793 2.320765

H -0.299749 -3.275870 0.786113

H 1.793734 -1.376507 1.692139

H 1.886436 -2.383069 0.370587

H 1.828721 -0.529274 -2.287174

H 2.787684 0.257966 -1.198637

H 1.765830 2.377830 -1.612882

H 2.113231 1.654075 -3.210819

H -0.229575 0.746090 -3.306512

H -0.268284 2.517804 -3.076350

H -0.803566 2.230691 -0.819784

H -1.709698 1.096091 -1.545287

O -0.002145 3.216139 2.032143

H 0.399924 3.401674 2.902181

H 0.431538 2.363784 1.697498

O -2.782824 -1.741804 -2.466401

H -2.754655 -2.249984 -3.297609

H -1.833690 -1.672311 -2.165413

O 2.666377 0.038889 2.726766

H 2.051663 0.593159 2.168012

H 2.402948 0.206812 3.650914

O 4.478038 -0.522619 -0.658336

H 4.812610 -0.291115 0.273857

H 5.220414 -0.323371 -1.258417

O -3.761465 -3.515960 2.419841

H -3.214664 -4.275464 2.146437

H -3.830682 -2.994814 1.577926

O 1.686565 -2.225004 -3.090170

H 2.282806 -2.599224 -2.387588

H 0.811803 -2.225514 -2.640428

O 5.208710 0.065890 1.807556

H 5.597142 -0.743554 2.190126

H 4.310327 0.122184 2.241967

O -3.705628 -2.013248 0.099558

H -3.384717 -2.352836 -0.771534

H -4.202367 -1.195162 -0.220725

O -1.384141 4.040317 -0.261982

H -0.514671 4.419802 -0.562022

H -1.196871 3.932233 0.697721

O 3.218139 -2.858199 -0.886184

H 3.826485 -2.059196 -0.798543

H 3.782682 -3.640839 -0.750684

O -2.372967 1.768201 2.261875

H -2.852172 1.867364 3.105463

H -1.572345 2.354349 2.340702

O -3.556990 2.283196 -0.205049

H -2.944355 2.998920 -0.491591

H -3.245177 2.089286 0.717163

O -4.628382 0.047931 -1.307341

H -3.996513 -0.350470 -1.951364

H -4.203077 0.896889 -1.000804

O 1.255755 4.582744 -0.252585

H 1.101242 4.265998 0.667714

H 1.588402 5.492769 -0.137930

**Configuration 05**

69

Tc 0.220263 -0.400106 0.000646

O -1.265310 -1.312569 -0.243538

O 1.759590 0.361622 0.372790

N -0.414594 1.243239 -1.242419

N 0.979595 -1.058157 -1.934969

N 0.870273 -2.101734 1.259015

N -0.475561 0.269384 1.968402

C 0.364417 1.242767 -2.514131

C 0.446666 -0.189433 -3.028759

C 0.177389 -2.028566 2.576801

C 0.142300 -0.574878 3.033636

H -0.350480 2.193003 -0.809966

H -1.438269 1.147915 -1.467130

H 1.371528 1.646439 -2.303036

H -0.118472 1.895081 -3.264684

H -0.559299 -0.553615 -3.298517

H 1.088346 -0.255353 -3.925067

H 0.729279 -2.036590 -2.121851

H 2.033611 -1.031024 -1.952861

H 1.904020 -2.075237 1.379854

H 0.666233 -3.002804 0.810835

H -0.849300 -2.406152 2.441950

H 0.676908 -2.662250 3.331011

H 1.169671 -0.210140 3.200166

H -0.410701 -0.480856 3.984944

H -1.512958 0.210010 2.028598

H -0.211027 1.253040 2.143202

O 4.308291 0.249117 0.219982

H 3.314833 0.422008 0.383087

H 4.801077 0.869430 0.789320

O -3.405690 -2.350822 0.768296

H -3.193141 -3.196062 1.207685

H -2.548041 -2.057222 0.297621

O -4.716821 1.563714 0.447926

H -5.215361 2.243331 0.936715

H -4.286886 0.994180 1.150730

O -3.413336 -0.067913 2.163102

H -3.760758 -0.151802 3.070958

H -3.506828 -0.982810 1.754864

O 2.092492 4.047516 0.698252

H 2.467798 4.903410 0.978200

H 1.786621 3.608532 1.542029

O -5.460676 0.098024 -1.820971

H -5.424582 -0.874397 -1.597794

H -5.444235 0.541795 -0.937558

O 3.826669 -2.211833 1.277346

H 4.330539 -2.409814 2.088749

H 4.146478 -1.311735 0.976614

O -5.399253 -2.548897 -1.103313

H -4.679593 -2.533681 -0.414040

H -6.213835 -2.633291 -0.573068

O 4.278259 -3.551124 -1.053297

H 4.150984 -3.185207 -0.133674

H 5.238597 -3.716757 -1.100208

O 3.810729 -1.114921 -2.214541

H 4.007939 -2.041115 -1.892478

H 4.182622 -0.556104 -1.495097

O 0.918781 2.864463 2.848546

H 0.327983 3.517290 3.273039

H 1.513807 2.583582 3.571162

O -3.150854 1.517679 -1.836330

H -3.868195 0.857311 -2.055872

H -3.512040 1.845875 -0.977424

O -0.406470 3.992688 -0.390024

H 0.509447 4.141116 -0.026984

H -0.979411 4.083251 0.394013

O 3.457626 2.757389 -1.439417

H 3.005850 3.164866 -0.661196

H 3.813113 1.925594 -1.068554

**Configuration 06**

69

Tc -0.126880 -0.117858 0.050356

O -1.530273 0.405301 -0.868428

O 1.302164 -0.541851 1.018186

N -1.401252 -0.947637 1.609839

N -0.314625 1.612423 1.402210

N 1.185336 0.588351 -1.542021

N 0.078114 -1.914068 -1.119328

C -1.711186 0.057116 2.671236

C -0.588873 1.086680 2.768629

C 1.214944 -0.409430 -2.649232

C 1.244083 -1.806475 -2.035430

H -0.918013 -1.787623 1.969664

H -2.304398 -1.291788 1.218095

H -1.880353 -0.431222 3.645930

H -2.650645 0.555498 2.377179

H -0.869139 1.900000 3.461669

H 0.334920 0.616303 3.142813

H -1.087642 2.241125 1.105345

H 0.500044 2.245489 1.400806

H 2.152264 0.710273 -1.169832

H 1.003406 1.547634 -1.905664

H 0.298634 -0.289455 -3.252137

H 2.085367 -0.242822 -3.308277

H 2.168879 -1.946080 -1.449214

H 1.210168 -2.585524 -2.817660

H -0.799900 -1.996641 -1.694277

H 0.126292 -2.734188 -0.481992

O 2.534458 -2.752269 1.850834

H 2.633777 -2.727717 2.822581

H 2.102504 -1.872894 1.624047

O -3.444137 2.190759 -1.017031

H -3.717452 2.392018 -1.932373

H -2.722857 1.485126 -1.089657

O -2.219643 -1.647203 -2.740592

H -3.013416 -2.147993 -2.383336

H -2.267835 -0.787939 -2.267079

O 0.003019 -3.579288 1.240393

H 0.959001 -3.506924 1.508330

H -0.217201 -4.522996 1.342215

O 4.979006 -1.563822 1.047197

H 4.224733 -2.176506 1.233896

H 4.638760 -0.710726 1.422080

O -5.171807 0.775530 0.543824

H -5.199131 1.256117 1.391832

H -4.604818 1.348571 -0.046905

O 0.752937 4.148415 0.371200

H -0.239812 4.212521 0.332547

H 1.040907 4.977602 0.794606

O -1.956336 3.868186 0.451304

H -2.523533 4.236370 1.153059

H -2.576609 3.387725 -0.170406

O -4.087719 -1.629047 0.741691

H -4.547155 -2.080671 1.474822

H -4.530539 -0.716626 0.681170

O 3.819128 1.616787 -0.917516

H 4.365493 0.831336 -1.222495

H 3.806298 1.510497 0.067278

O -4.345202 -2.905743 -1.636301

H -5.143837 -2.516027 -2.038971

H -4.306235 -2.474740 -0.733649

O 3.575247 0.744498 1.681460

H 2.682334 0.312919 1.540989

H 3.513482 1.211124 2.535670

O 5.197538 -0.643988 -1.463409

H 5.114049 -1.093659 -0.564316

H 4.748773 -1.249548 -2.080890

O 1.838914 3.322409 -2.037465

H 1.460873 3.719854 -1.210055

H 2.640200 2.849891 -1.701637

**Configuration 07**

69

Tc -0.157933 -0.213364 0.171810

O 0.109475 -1.978375 -0.015945

O -0.564304 1.459364 0.419123

N 1.223585 -0.163519 1.856854

N -1.531395 -0.670452 1.845993

N -1.450465 -0.274417 -1.592661

N 1.245291 0.312344 -1.387152

C 0.621137 -0.832257 3.042177

C -0.843276 -0.428262 3.148005

C -0.612732 -0.403474 -2.817638

C 0.560637 0.559298 -2.690136

H 1.424629 0.839472 2.052590

H 2.136149 -0.609498 1.635395

H 1.164828 -0.573064 3.968311

H 0.712492 -1.920511 2.891063

H -1.340935 -0.974139 3.969047

H -0.918055 0.650344 3.368113

H -1.829982 -1.659291 1.757813

H -2.399927 -0.103989 1.834541

H -1.970689 0.625855 -1.644471

H -2.193058 -1.016672 -1.584571

H -0.247644 -1.443168 -2.881600

H -1.204942 -0.185180 -3.725224

H 0.197157 1.601602 -2.688225

H 1.266272 0.448151 -3.532101

H 1.982936 -0.410625 -1.491623

H 1.770256 1.172084 -1.093569

O -1.587497 3.767313 -0.201678

H -2.118684 4.164280 0.515295

H -1.239227 2.898347 0.178035

O 0.714833 -3.518247 -2.307660

H 1.622047 -3.194131 -2.459473

H 0.459696 -3.040293 -1.482272

O 1.878811 -3.776731 1.008338

H 1.508113 -4.170245 1.819832

H 1.142629 -3.216019 0.635186

O 2.786360 2.569972 -0.565342

H 3.684344 2.236704 -0.874455

H 2.772269 2.441294 0.418315

O 3.817050 -1.078946 -1.384396

H 4.230741 -1.791051 -1.906796

H 3.839860 -1.399102 -0.428466

O -3.672200 -2.053308 -1.449933

H -4.171576 -1.251932 -1.122199

H -3.346376 -2.516486 -0.640666

O -2.226406 -3.216021 0.669907

H -2.173874 -4.162828 0.896895

H -1.328192 -2.979776 0.311737

O 1.983415 2.646051 2.068957

H 1.524987 3.413886 1.600045

H 2.559601 3.061863 2.736338

O -3.068423 2.181613 -1.857473

H -3.080840 2.533240 -2.766744

H -2.612267 2.884300 -1.310223

O -4.005521 0.943190 1.813371

H -3.813737 1.899503 1.872440

H -4.593034 0.769000 2.574129

O 3.577614 -1.777297 1.162419

H 3.032291 -2.630465 1.191359

H 4.338950 -1.917180 1.754867

O 5.028016 1.367884 -1.419436

H 4.661582 0.437085 -1.446955

H 5.686067 1.334160 -0.700090

O -4.869575 0.326946 -0.763156

H -4.340087 1.022070 -1.229739

H -4.678084 0.527898 0.185969

O 1.105185 4.533181 0.383073

H 1.676181 4.035379 -0.253949

H 0.179851 4.371536 0.071194

**Configuration 08**

69

Tc -0.135463 -0.573593 0.292981

O 1.485665 -0.205637 0.887644

O -1.784022 -1.008639 -0.179479

N 0.613163 -2.068912 -1.084250

N 0.105076 0.630885 -1.497364

N -0.940074 0.848614 1.764221

N -0.405801 -1.893917 2.018794

C 0.315452 -1.635952 -2.478257

C 0.715277 -0.169291 -2.606403

C -0.934100 0.218517 3.117712

C -1.328679 -1.250666 2.993339

H 0.189147 -2.986065 -0.844246

H 1.643767 -2.188794 -0.969475

H -0.764650 -1.771496 -2.652941

H 0.861902 -2.256210 -3.211277

H 1.812347 -0.065482 -2.522976

H 0.409210 0.233310 -3.588297

H 0.686055 1.503110 -1.401675

H -0.828641 1.003440 -1.768123

H -1.920725 1.143758 1.552298

H -0.413563 1.746007 1.805296

H 0.084917 0.300854 3.534019

H -1.621281 0.748586 3.800945

H -2.351506 -1.337061 2.590784

H -1.297745 -1.756258 3.974352

H 0.513781 -2.044930 2.452534

H -0.729543 -2.825653 1.689979

O 2.626770 2.306176 0.901812

H 2.213647 1.402069 0.910566

H 3.602089 2.103459 0.847075

O 3.908935 -1.124935 1.440791

H 4.025268 -1.500326 2.333692

H 2.961736 -0.785151 1.397875

O -4.330711 -0.254854 0.044615

H -3.395326 -0.616254 -0.031236

H -4.889607 -0.997745 0.339578

O -0.815300 -4.196491 0.332012

H -1.610143 -4.067732 -0.266578

H -0.651213 -5.156597 0.345826

O 3.501022 -2.379089 -0.903058

H 3.767943 -2.105368 0.018994

H 3.904794 -3.255119 -1.044352

O -2.140588 2.375407 -2.014469

H -2.000654 2.693063 -2.926642

H -3.093422 2.037160 -2.020147

O -0.611526 4.302467 -0.662797

H -1.275552 3.640555 -0.983643

H -0.401519 4.039020 0.268674

O 1.626239 3.027087 -1.584833

H 2.101806 2.871666 -0.728447

H 0.848569 3.596597 -1.313182

O -4.597651 1.335578 -2.126346

H -4.622891 0.690104 -1.366221

H -4.559836 0.761845 -2.914867

O 0.399370 3.442824 1.790536

H 1.350357 3.198962 1.604898

H 0.407211 3.924694 2.637562

O -3.635185 1.879905 1.564510

H -4.060541 1.112073 1.097965

H -3.967184 1.809033 2.478787

O -2.690802 -3.330255 -1.349892

H -3.632710 -3.484383 -1.148757

H -2.504502 -2.425297 -0.984165

O 4.992930 1.133771 0.434946

H 4.791497 0.283079 0.919586

H 5.919128 1.349171 0.649011

O 4.252344 0.052623 -2.148716

H 4.067033 -0.858878 -1.818226

H 4.541276 0.517837 -1.329354

**Configuration 09**

69

Tc 0.295700 0.215423 0.071372

O -1.452868 0.233111 0.035518

O 2.066904 0.170645 0.116684

N 0.227281 -1.727735 -0.962286

N 0.249019 -1.171108 1.758107

N 0.311828 2.129225 1.108946

N 0.507154 1.580652 -1.613068

C 0.334035 -2.857702 0.006723

C -0.330039 -2.467177 1.321074

C 0.405255 3.280363 0.156241

C 1.110231 2.852899 -1.125436

H 0.982298 -1.849077 -1.664636

H -0.683192 -1.774399 -1.461540

H 1.407126 -3.056412 0.169490

H -0.131137 -3.773853 -0.396034

H -1.414278 -2.354871 1.159616

H -0.173611 -3.253221 2.083000

H -0.207936 -0.813763 2.612994

H 1.248843 -1.318701 2.029163

H 1.093784 2.098737 1.795024

H -0.569747 2.245332 1.636468

H -0.624951 3.596592 -0.073193

H 0.925305 4.135253 0.621848

H 2.181710 2.677074 -0.939614

H 1.027936 3.647624 -1.889070

H -0.418916 1.794682 -2.061528

H 1.123935 1.177862 -2.342042

O -3.880512 -0.120855 -0.860287

H -4.415255 -0.679865 -0.236593

H -2.988634 -0.000959 -0.399006

O 3.948725 -1.701914 -0.143784

H 3.243826 -0.999906 -0.044848

H 3.646233 -2.146708 -0.980244

O 4.393904 0.932181 -1.128312

H 3.601159 0.941766 -0.531267

H 4.718448 0.018986 -0.937213

O 2.660273 -2.201165 -2.505850

H 2.744522 -2.832898 -3.243128

H 2.750869 -1.287797 -2.914459

O -2.437207 -1.956200 -2.205817

H -2.675774 -2.067190 -3.144004

H -3.059351 -1.254257 -1.849090

O 2.247721 1.394802 3.214183

H 1.492639 1.004263 3.721166

H 2.655552 0.598381 2.809775

O -2.524363 2.907289 1.704935

H -2.996301 2.312580 2.319636

H -2.662139 3.794236 2.090547

O -1.961273 2.423148 -2.772789

H -2.646787 2.551573 -2.044130

H -2.331875 1.688042 -3.295912

O -0.038671 0.212512 4.365398

H -0.731517 0.831937 4.665363

H 0.111904 -0.363852 5.139071

O -3.825090 2.613914 -0.836431

H -3.387224 2.718815 0.044267

H -4.060501 1.647849 -0.850375

O -3.091441 -3.807181 -0.175304

H -2.862434 -3.276089 -0.976426

H -3.803615 -3.265143 0.234007

O 2.781285 0.381609 -3.180184

H 3.114846 0.706583 -4.036499

H 3.471048 0.660527 -2.497399

O 3.087656 -1.535129 2.505844

H 3.480498 -1.806222 1.635211

H 3.188685 -2.329145 3.064837

O -5.112425 -1.965339 0.790042

H -6.031404 -2.217239 0.577082

H -5.134491 -1.769306 1.746401

**Configuration 10**

69

Tc -0.425095 -0.040678 0.122951

O -1.896713 -0.484854 -0.752927

O 1.122354 0.163970 0.941329

N -0.393398 -2.146041 0.818256

N -1.447684 0.148846 2.020637

N -0.630416 2.013858 -0.514281

N 0.669097 -0.098149 -1.786968

C -1.283381 -2.291276 2.014167

C -1.172567 -1.037839 2.874486

C -0.161214 2.193797 -1.920034

C 1.050464 1.299552 -2.139841

H 0.577895 -2.400341 1.069645

H -0.721088 -2.789841 0.080917

H -1.015740 -3.193043 2.592930

H -2.321854 -2.406633 1.657457

H -1.876471 -1.089263 3.724791

H -0.153607 -0.933913 3.285551

H -2.471452 0.227442 1.826006

H -1.160454 1.030073 2.508080

H -0.079277 2.636788 0.119675

H -1.627392 2.295022 -0.437059

H -0.972681 1.881451 -2.597233

H 0.074644 3.253114 -2.122591

H 1.879811 1.608675 -1.482545

H 1.401911 1.362098 -3.185762

H 0.031982 -0.443286 -2.535379

H 1.539323 -0.679668 -1.806956

O -2.461035 -3.088522 -1.036827

H -2.610110 -3.392540 -1.951239

H -2.311001 -2.106579 -1.117758

O 2.429670 -2.031662 1.718419

H 2.597186 -2.033179 2.679941

H 2.107934 -1.106260 1.506578

O 3.106762 2.048704 1.130516

H 3.685278 1.843171 0.344582

H 2.493261 1.271784 1.158688

O -3.422062 0.484043 -2.646004

H -2.946351 -0.008530 -1.905981

H -4.246354 -0.017290 -2.797657

O -4.224218 0.392606 1.240659

H -4.098281 1.113189 0.557623

H -4.831519 0.774346 1.900959

O -1.203874 -0.538150 -4.034531

H -0.918091 0.046907 -4.760169

H -2.051174 -0.130784 -3.722974

O -3.583435 2.272352 -0.622095

H -3.664200 1.777426 -1.487290

H -4.103338 3.089480 -0.735929

O 4.456493 -2.555356 0.081244

H 3.724618 -2.426924 0.761081

H 4.678520 -3.504534 0.103631

O 3.303444 -1.163550 -2.036478

H 3.673729 -1.809197 -1.383990

H 3.761159 -0.324552 -1.773433

O -4.529172 -2.427950 0.827241

H -4.440477 -1.445598 0.852771

H -3.914018 -2.702917 0.107689

O 6.299849 -0.589293 0.273450

H 6.993521 -0.828536 -0.370046

H 5.697751 -1.389974 0.275363

O 4.626022 1.074801 -0.929862

H 5.330630 0.510627 -0.462251

H 5.126489 1.669799 -1.519240

O -0.569783 2.623511 3.243418

H -1.341769 3.219569 3.229122

H 0.050973 3.039611 2.582328

O 1.004735 3.591382 1.224815

H 1.907541 3.128259 1.140309

H 1.166298 4.542463 1.087760

**[TcO4]-**

**Configuration 01**

47

Tc -0.558136 -0.333455 -0.079491

O -0.875991 0.870921 1.108385

O 0.674449 0.239689 -1.132125

O -0.031181 -1.783285 0.728323

O -1.990524 -0.679518 -0.985692

O -0.643181 -2.988490 -2.611255

H -1.296671 -2.264364 -2.560142

H 0.192115 -2.507094 -2.826251

O -3.756066 1.604089 -1.224174

H -3.314344 0.745025 -1.393955

H -3.995137 1.532381 -0.255727

O 1.731948 -1.455284 -2.970433

H 1.364130 -0.701965 -2.440028

H 1.942224 -1.068807 -3.842025

O 1.523103 1.886353 2.274782

H 1.981178 2.251688 1.469165

H 0.711839 1.480856 1.892946

O -1.482742 2.826783 -2.312185

H -2.292070 2.525186 -1.829042

H -0.897161 3.173471 -1.594422

O 4.324438 0.824931 0.022815

H 4.137507 0.525971 0.963989

H 4.135260 0.003552 -0.520909

O -4.005634 -1.485354 0.953472

H -3.479902 -1.386400 0.130429

H -3.337163 -1.858942 1.596235

O 3.889543 -1.586557 -1.163391

H 3.441527 -1.973330 -0.368240

H 3.188272 -1.610675 -1.861611

O -2.037306 -2.455710 2.595639

H -1.248033 -2.376080 2.006932

H -1.845866 -1.821610 3.311684

O 0.222012 3.834068 -0.307500

H -0.122069 3.536476 0.554953

H 1.152671 3.489428 -0.305892

O 3.522291 0.007354 2.490049

H 3.150565 -0.855032 2.175441

H 2.736374 0.621914 2.520176

O -4.417831 1.132323 1.399803

H -4.296234 0.134998 1.306746

H -5.385196 1.236917 1.466006

O 2.590768 -2.293456 1.206555

H 1.614339 -2.181422 1.049362

H 2.683642 -3.174703 1.614351

O 2.796934 2.902622 0.038121

H 3.414078 3.587254 0.357051

H 3.383719 2.062058 -0.088604

**Configuration 02**

47

Tc -0.262512 -0.763243 -0.049314

O 1.270237 -1.131797 -0.753661

O -1.109966 0.312614 -1.105169

O -1.168175 -2.222118 0.127281

O -0.044297 -0.006820 1.491039

O -3.073052 -3.083980 -1.730400

H -2.532272 -3.363056 -2.493573

H -2.402202 -2.938894 -1.020601

O -0.974312 3.088929 -0.821590

H -1.090166 2.126923 -1.025998

H -0.756877 3.076089 0.144542

O -0.669669 2.587772 1.916431

H -0.546053 2.955024 2.811675

H -0.471781 1.615708 1.981640

O 3.787500 -2.508456 -0.501287

H 2.866719 -2.203721 -0.667633

H 3.961463 -2.117512 0.392526

O -3.722126 -0.432520 -2.056317

H -2.818768 -0.058217 -1.968305

H -3.550983 -1.414455 -1.995245

O -3.200565 -1.460747 2.145612

H -3.696471 -0.826935 1.549391

H -2.674875 -1.977771 1.504367

O -3.349961 2.788886 0.856851

H -2.577826 2.685392 1.461045

H -2.898083 3.069036 0.030955

O 2.642636 0.817034 -2.392843

H 2.240719 1.699285 -2.172115

H 2.066694 0.167386 -1.932261

O 1.918180 -1.738040 2.666873

H 1.246227 -1.035636 2.550893

H 2.731612 -1.312544 2.302722

O 2.328779 2.584471 0.995848

H 2.173369 2.892268 0.069332

H 1.440813 2.680254 1.394341

O -4.503161 0.277251 0.495061

H -4.095134 1.177522 0.605267

H -4.263075 0.015663 -0.437876

O 1.589311 3.241032 -1.623973

H 1.822112 4.076562 -2.068968

H 0.600841 3.287805 -1.449302

O 4.254281 -0.661428 1.542075

H 4.450086 -0.190430 0.665763

H 5.119959 -0.735623 1.984048

O 4.809270 0.039310 -0.948819

H 4.605244 -0.926329 -1.061151

H 4.057451 0.464511 -1.459079

**Configuration 03**

47

Tc 0.339310 -0.563567 -1.397772

O 0.175704 0.256693 0.116052

O -0.733303 0.162776 -2.539706

O 1.948988 -0.438643 -1.982133

O -0.060793 -2.238794 -1.190389

O -1.589281 0.204902 2.252408

H -2.387940 -0.334675 1.976600

H -1.049124 0.237919 1.425316

O 1.212357 2.157620 1.998016

H 0.327431 2.499955 2.363540

H 0.918920 1.476116 1.350147

O -2.742093 1.725477 -1.638163

H -3.152511 2.230815 -2.366582

H -2.025820 1.189458 -2.080105

O 1.404627 3.637450 -0.319404

H 1.403863 3.282622 0.609072

H 2.069581 3.018624 -0.740196

O 3.357540 1.845891 -1.018395

H 3.482096 1.435066 -0.107063

H 2.986112 1.097871 -1.534538

O -1.317724 3.653438 -0.086204

H -0.354245 3.592540 -0.347752

H -1.779560 2.963204 -0.620972

O 2.258662 -3.563203 -0.294677

H 2.037991 -4.406809 0.142905

H 1.391293 -3.251453 -0.649051

O -1.259355 2.929865 2.529287

H -1.584513 1.991635 2.519360

H -1.362257 3.219659 1.570002

O -1.481032 -3.336124 1.027802

H -1.046048 -3.056179 0.190313

H -2.271897 -2.736451 1.082495

O 3.566987 0.786384 1.481051

H 2.866367 1.322384 1.921111

H 3.205636 -0.150805 1.545346

O 2.568968 -1.709130 1.778575

H 1.650428 -1.764305 2.177865

H 2.533540 -2.359023 1.029687

O -4.420981 -0.308340 -0.886068

H -3.844891 0.473553 -1.122567

H -5.299432 0.084762 -0.726864

O -3.494654 -1.443561 1.298907

H -4.256784 -1.667522 1.865041

H -3.890187 -1.019392 0.461794

O 0.072182 -1.998081 2.862635

H -0.441617 -2.575404 2.226988

H -0.451151 -1.157734 2.825576

**Configuration 04**

47

Tc -1.117097 -1.495882 0.239797

O -0.334401 -0.078783 -0.341453

O -0.898601 -2.766421 -0.897549

O -0.409987 -1.957017 1.758733

O -2.805409 -1.170562 0.471462

O 2.388816 -2.220335 1.341648

H 1.461016 -2.287334 1.663643

H 2.574210 -1.250615 1.414352

O -3.435129 1.466396 0.909841

H -4.300382 1.587994 1.345000

H -3.328164 0.481104 0.825543

O 3.107479 -0.563328 -2.362055

H 2.607063 -1.364157 -2.033292

H 3.799599 -0.433029 -1.659454

O -0.497488 2.236043 -1.785504

H -0.331067 2.866224 -1.021186

H -0.463157 1.357828 -1.327061

O 0.390288 0.476872 3.072481

H 1.228478 0.534999 2.546503

H 0.039270 -0.408969 2.827253

O 2.636783 2.653212 0.203785

H 2.560627 2.391844 -0.775694

H 1.764473 3.101446 0.381916

O -3.507753 -0.658960 -2.352241

H -3.426825 0.330297 -2.241858

H -3.630760 -0.952340 -1.427820

O 2.013241 -2.823819 -1.297007

H 1.039025 -2.934554 -1.334970

H 2.185268 -2.638735 -0.327415

O -1.247730 2.506193 2.306783

H -0.687469 1.730378 2.606202

H -2.042588 2.105177 1.868761

O 2.252051 1.974231 -2.341759

H 2.449146 0.986331 -2.377342

H 1.264109 2.045144 -2.328781

O 2.858668 0.554999 1.616849

H 2.726633 1.426345 1.032347

H 3.422599 0.837918 2.362759

O 0.108147 3.656520 0.430343

H -0.055883 4.615783 0.489519

H -0.439872 3.227906 1.194816

O 4.876493 -0.094517 -0.273695

H 5.249756 0.790124 -0.448326

H 4.208096 0.081708 0.436973

O -3.265767 2.050153 -1.858848

H -3.390601 1.966358 -0.880899

H -2.285049 2.200769 -1.937239

**Configuration 05**

47

Tc -0.025006 -1.343222 -0.386937

O -1.302586 -2.363239 -0.946188

O -0.233568 -1.058140 1.297444

O 1.516339 -2.104657 -0.645035

O -0.067776 0.139443 -1.255748

O 3.685888 -0.690060 -1.520876

H 2.934577 -1.250912 -1.184673

H 4.048871 -1.186372 -2.278171

O -2.394910 -0.274980 3.178223

H -1.645127 0.386473 3.211806

H -1.962321 -1.017987 2.712437

O 0.931394 2.701294 -1.090406

H 0.443922 1.845065 -1.176702

H 1.840962 2.483576 -1.474581

O -3.870893 -1.425522 -0.842656

H -2.981610 -1.872660 -0.856636

H -4.513659 -2.137116 -1.022061

O 1.229028 -4.468717 0.899376

H 1.563461 -3.743752 0.325622

H 0.772495 -5.042867 0.256319

O -0.032622 1.058058 3.131739

H 0.203629 1.846883 2.575385

H 0.225341 0.313895 2.542861

O -4.177779 0.463471 1.241280

H -4.127150 -0.288589 0.601937

H -3.550729 0.206045 1.975956

O -3.564120 0.660360 -2.618737

H -3.750614 -0.139703 -2.056931

H -4.454258 0.995250 -2.836168

O 3.293827 1.961081 -2.080885

H 3.423902 0.998923 -1.848814

H 3.208846 1.948462 -3.052710

O 2.847931 0.834493 1.960330

H 2.338892 1.679145 1.810917

H 2.713820 0.659871 2.909699

O 5.258339 0.392971 0.616855

H 4.839903 -0.092612 -0.127963

H 4.469775 0.608158 1.172196

O -2.825275 2.172066 -0.381111

H -3.037883 1.714212 -1.234877

H -3.322924 1.623311 0.291017

O 1.155432 2.915593 1.516664

H 1.341278 3.842491 1.754544

H 1.042699 2.903734 0.504835

O -1.281051 4.438532 -0.638908

H -0.460311 4.001269 -0.952636

H -1.871299 3.657971 -0.475213

**Configuration 06**

47

Tc -0.087100 -0.380444 -0.434873

O -1.793529 -0.650948 -0.613374

O 0.289883 1.214682 -0.996632

O 0.342336 -0.516941 1.225275

O 0.779373 -1.537694 -1.377037

O -3.209129 1.538696 0.695318

H -2.601396 2.301684 0.493438

H -2.772196 0.783745 0.240412

O 2.729813 0.986373 2.069614

H 2.723746 1.599070 1.275805

H 1.826762 0.605618 2.053222

O 3.731581 -1.075887 -1.425437

H 2.786348 -1.261451 -1.604699

H 3.816158 -1.208037 -0.419854

O -3.694799 -0.114692 -2.647119

H -3.426228 0.772922 -2.952175

H -2.940845 -0.392018 -2.075621

O -1.221942 3.334929 0.021675

H -1.462773 3.980659 -0.670657

H -0.674047 2.660427 -0.453952

O 1.860999 -2.948021 1.981360

H 1.599381 -3.455977 1.161617

H 1.198125 -2.226771 2.006631

O 2.639220 2.536454 -0.170347

H 1.830349 2.148503 -0.576683

H 3.375177 2.218961 -0.792869

O -4.149933 -1.854778 0.769984

H -4.694810 -1.130357 0.338437

H -3.314734 -1.810104 0.260548

O 4.400624 1.463627 -1.821547

H 4.142822 0.487975 -1.708273

H 4.106781 1.676599 -2.726979

O 1.141360 -4.143923 -0.376108

H 1.040841 -3.315170 -0.900930

H 0.227726 -4.481557 -0.312686

O -3.032515 -0.314671 2.839296

H -3.471226 -0.951122 2.216818

H -3.076126 0.512013 2.306245

O 1.159971 4.415148 1.353610

H 1.799655 3.922125 0.791333

H 0.295769 4.109963 0.999055

O 3.938061 -1.319852 1.204951

H 3.243899 -1.976553 1.500602

H 3.572497 -0.449993 1.540192

O -5.372606 0.256718 -0.471804

H -4.911669 0.143982 -1.347182

H -4.804818 0.940200 -0.035656

**Configuration 07**

47

Tc -0.076070 -0.403446 -0.393137

O -1.783924 -0.675755 -0.560332

O 0.301613 1.186062 -0.968721

O 0.363848 -0.533310 1.264659

O 0.785442 -1.565647 -1.332348

O -3.267784 1.592348 0.500265

H -2.687247 2.362358 0.252409

H -2.785725 0.826362 0.114467

O 2.752188 1.001912 2.065416

H 2.720930 1.630569 1.284374

H 1.854618 0.608138 2.062505

O 3.729094 -0.992266 -1.480213

H 2.788959 -1.204862 -1.654294

H 3.826791 -1.138007 -0.477628

O -3.715035 -0.484768 -2.614117

H -3.507239 0.361948 -3.053431

H -2.943965 -0.621499 -2.014397

O -1.285570 3.364268 -0.232431

H -1.463283 3.962317 -0.983916

H -0.711507 2.653355 -0.615041

O 1.957517 -2.927434 1.990027

H 1.688959 -3.448875 1.181075

H 1.276815 -2.223607 2.028787

O 2.594949 2.594350 -0.139310

H 1.794677 2.181402 -0.538070

H 3.331064 2.300447 -0.772865

O -4.071788 -1.816510 0.981342

H -4.649650 -1.167014 0.479706

H -3.245183 -1.795539 0.456438

O 4.354895 1.568610 -1.824690

H 4.105678 0.589169 -1.734750

H 4.059230 1.801268 -2.724730

O 1.224749 -4.160582 -0.343223

H 1.087032 -3.337346 -0.868460

H 0.324667 -4.529748 -0.263772

O -2.997348 0.007472 2.837087

H -3.413202 -0.718859 2.303847

H -3.076907 0.757297 2.203391

O 0.959345 4.391717 1.329872

H 1.650742 3.940317 0.795104

H 0.133763 4.129099 0.865489

O 3.978626 -1.265620 1.143183

H 3.303962 -1.932627 1.460167

H 3.616030 -0.403034 1.500850

O -5.385858 0.093820 -0.479748

H -4.928422 -0.108213 -1.341002

H -4.840256 0.844032 -0.135108

**Configuration 8**

47

Tc 0.163223 -0.727157 0.085104

O 1.109189 -2.008071 -0.567043

O -0.779000 -0.023397 -1.179381

O -0.894910 -1.360475 1.295053

O 1.188168 0.475552 0.795799

O 4.882519 -1.465103 -0.179607

H 5.827210 -1.607565 -0.373071

H 4.377896 -2.060171 -0.822126

O 0.435044 3.193478 0.891279

H 0.751750 2.287054 1.109091

H 0.698221 3.269617 -0.079297

O -4.710549 0.258057 -1.434858

H -4.032171 0.992878 -1.434441

H -4.786139 -0.002927 -0.465185

O -2.747881 0.603953 2.468994

H -2.036196 -0.025575 2.221239

H -2.510227 1.443089 1.985943

O -2.679845 2.106231 -1.504270

H -1.944883 1.456353 -1.563822

H -2.560104 2.470069 -0.583481

O 3.908606 0.975886 0.545686

H 2.938584 0.788774 0.578328

H 4.298924 0.153653 0.134439

O 3.875529 3.219157 -0.921462

H 3.966503 2.366853 -0.390882

H 3.871442 3.909155 -0.231050

O -3.034504 -1.710596 -2.082313

H -2.188200 -1.221584 -1.993385

H -3.719458 -0.978586 -1.914535

O 1.297000 3.161649 -1.646745

H 1.127466 3.978261 -2.151423

H 2.287565 3.193447 -1.450359

O -3.241765 -2.813157 0.385824

H -3.146458 -2.489448 -0.562683

H -2.413900 -2.489270 0.803822

O 3.379210 -3.027593 -1.717262

H 2.501228 -2.686047 -1.411536

H 3.432732 -3.906383 -1.295920

O 3.740338 -1.401479 2.366333

H 3.741622 -0.428625 2.254207

H 4.205014 -1.661086 1.534697

O -2.147626 2.887411 1.057816

H -1.137568 3.063052 1.011639

H -2.540606 3.708233 1.409448

O -4.783615 -0.649022 1.112639

H -4.095039 -0.135798 1.624782

H -4.301060 -1.499540 0.904262

**Configuration 09**

47

Tc 0.643374 -0.720999 -0.215896

O -0.709944 0.318789 -0.345311

O 1.926681 -0.117897 -1.204164

O 1.112591 -0.764202 1.453800

O 0.161417 -2.301736 -0.744235

O 4.630767 -0.269442 -1.868358

H 4.730052 -1.175004 -2.218437

H 3.653353 -0.181962 -1.766493

O -1.642469 2.434572 -1.794250

H -2.515625 2.406464 -1.312788

H -1.192501 1.673411 -1.350105

O -2.299724 -1.789107 -2.300630

H -1.513539 -2.146324 -1.834650

H -2.840598 -1.391609 -1.565736

O -1.790290 2.614700 1.987383

H -2.503528 2.351397 1.348920

H -1.480087 1.753738 2.363154

O -0.994175 0.105317 3.016806

H -0.826299 0.055704 3.976906

H -0.148214 -0.192944 2.591386

O 3.189554 1.208370 2.076295

H 2.893900 1.791048 1.313313

H 2.451571 0.566413 2.138586

O 4.754148 -0.832372 0.937996

H 4.802667 -0.597093 -0.019246

H 4.280030 -0.053416 1.330360

O -2.795036 -1.728856 1.944194

H -2.186966 -1.081561 2.387533

H -2.208749 -2.504097 1.708828

O -1.174094 -3.797648 1.197553

H -0.484008 -3.946586 1.871467

H -0.672194 -3.412486 0.437598

O 2.349666 2.631541 -0.069435

H 1.418981 3.016243 0.029585

H 2.240918 1.889687 -0.698617

O -0.091227 3.710777 0.171187

H -0.608104 3.443013 -0.631634

H -0.643935 3.312409 0.910271

O -1.057509 0.292199 -3.690581

H -1.366773 1.098008 -3.220385

H -1.549340 -0.432967 -3.220476

O -3.638196 1.949183 -0.008709

H -3.757154 0.947992 -0.084481

H -4.540492 2.313400 0.053100

O -3.804024 -0.707062 -0.215957

H -3.404808 -1.111030 0.646184

H -4.718724 -1.045889 -0.249277

**Configuration 10**

47

Tc 0.724325 -0.701708 0.517818

O 1.011399 -1.826267 -0.756326

O -0.050717 -1.484055 1.838429

O 2.248368 -0.045548 1.033681

O -0.301445 0.566948 -0.054013

O -2.303488 0.500161 2.816518

H -1.463986 -0.000324 2.816061

H -2.041026 1.449087 2.620133

O -2.376955 -3.062719 1.033170

H -1.602922 -2.708706 1.520656

H -1.985953 -3.278683 0.130212

O -2.782939 0.280459 -1.318930

H -1.842714 0.356581 -1.027540

H -3.233825 -0.098984 -0.464376

O -0.789816 3.259949 -0.181340

H -1.604831 3.250181 -0.780145

H -0.547887 2.301200 -0.142182

O 3.734544 -0.723319 -1.347833

H 3.426160 -0.207341 -0.569457

H 2.953506 -1.292204 -1.522573

O 3.096318 2.616762 1.026252

H 2.822561 1.674340 1.136896

H 4.055750 2.556747 0.859184

O -1.253267 -3.529757 -1.378687

H -0.375066 -3.103179 -1.272193

H -1.727668 -2.914882 -2.016923

O -1.746844 3.123839 2.358238

H -1.387368 3.266439 1.432792

H -2.637813 3.519165 2.317202

O 4.140674 -2.355287 1.075377

H 4.242327 -1.978639 0.173248

H 3.771955 -1.587485 1.554895

O 1.802765 3.437189 -1.282405

H 0.869046 3.527758 -0.965530

H 2.293067 3.177360 -0.455882

O -3.749474 -0.724918 0.862803

H -3.313017 -1.630158 0.897584

H -3.270706 -0.226998 1.590587

O 1.977810 1.182664 -2.873402

H 2.727229 0.686795 -2.482934

H 1.924790 2.001715 -2.304646

O -2.530264 -1.804435 -3.022536

H -2.679239 -1.002373 -2.436448

H -1.877854 -1.490111 -3.676153

O -2.985039 2.952998 -1.700997

H -2.725035 3.051953 -2.636479

H -3.048473 1.956891 -1.586162