

## *Supporting Information*

# **INVESTIGATION OF IRON RELEASE FROM THE N- AND C- LOBES OF HUMAN SERUM TRANSFERRIN BY QUANTUM CHEMICAL CALCULATIONS**

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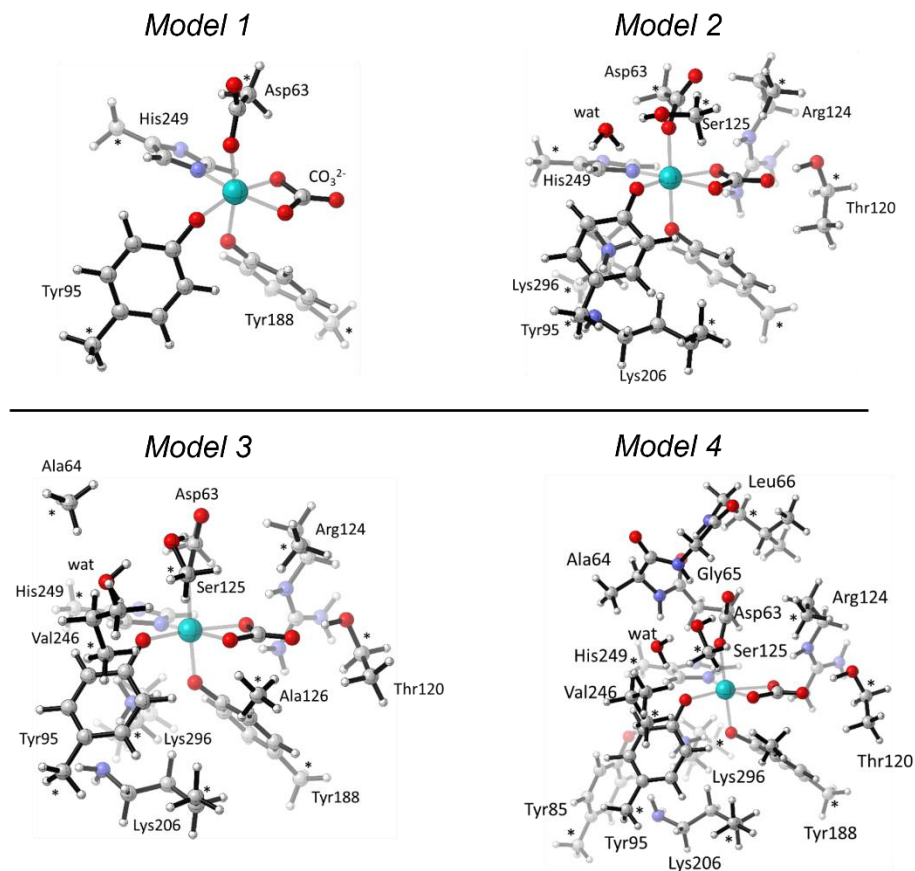
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## 1. The physiological pH models of the N- and C-lobe of hTf

To find out the optimum physiological model, the size of the cluster model is enlarged step by step starting from a basic model. This model (Model 1, Figure S1) includes iron and the first shell residues only and consists of 56 atoms. The all-atom RMSD value with respect to the crystal structure is calculated as 1.057 Å (Table S1). In Model 2, some of the second shell residues (Thr 120, Arg 124, Lys 206, Lys 296 and a water molecule bridging between Asp 63 and Tyr 95) are included and the RMSD value decreased to 0.877 Å. Next, all the residues within 6 Å around iron are included in Model 3 and the RMSD value drastically decreased (0.041 Å) that might point out to the suitability of the cluster size. To further confirm the convergence of the size of the cluster, a larger model (Model 4) consisting of 194 atoms is optimized and the RMSD value is calculated as 0.014 Å. Ultimately, Model 3 is chosen as the model for the iron-binding site at the physiological pH that compromise between the size and the efficiency. The corresponding model for C-lobe is constructed with a cluster size of 146 atoms (TfC<sup>Phys</sup>, Fig. 1). The RMSD value is calculated as low as 0.002 Å with respect to the C-lobe of the crystal structure. Thus, TfN<sup>Phys</sup> and TfC<sup>Phys</sup> are chosen to further assess the release of iron in hTf.



**Figure S1.** Optimized geometries of the physiological pH model with different cluster size.

**Table S1.** RMSD Values for different sizes of N-Lobe in physiologic environment.

|          | Model 1 | Model 2 | Model 3 | Model 4 |
|----------|---------|---------|---------|---------|
| Atom #   | 56      | 124     | 144     | 194     |
| RMSD (Å) | 1.057   | 0.877   | 0.041   | 0.014   |

## 2. The structural changes upon the protonation of the first coordination shell residues

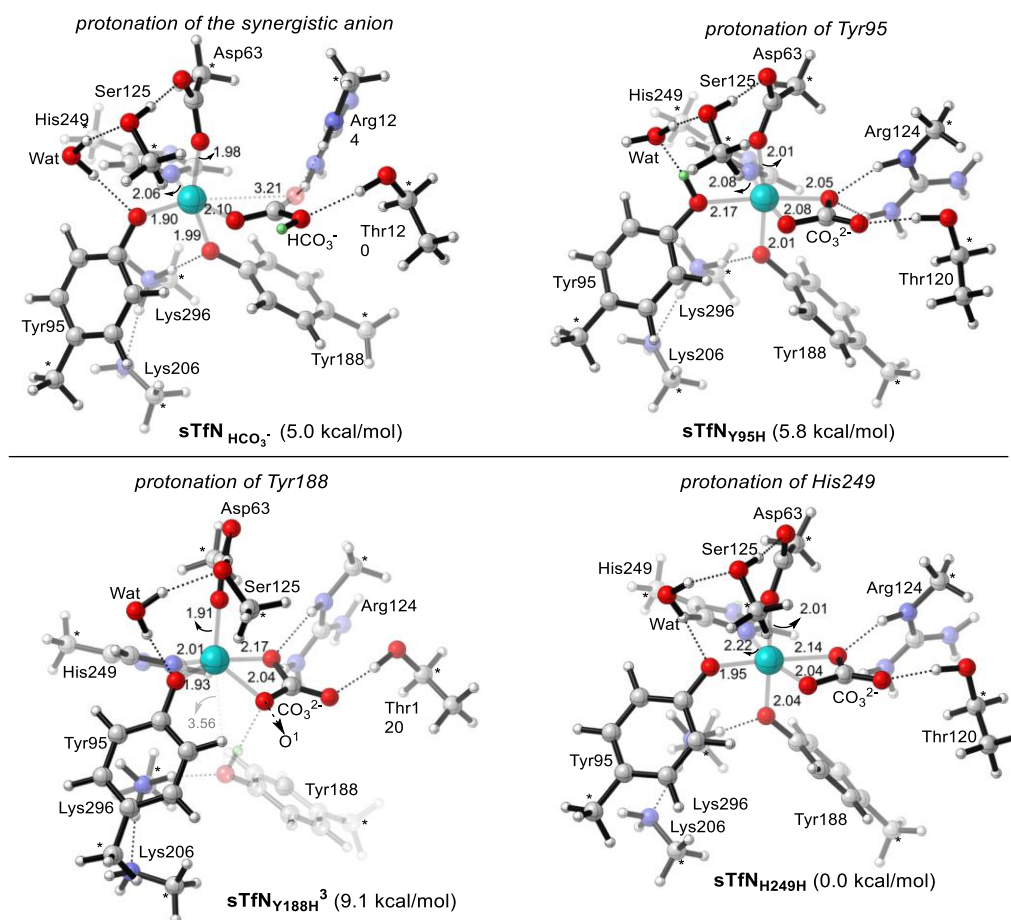
In this part of study, we have considered the protonation of each residue of the first coordination shell (His249, Tyr95, Tyr188 and the synergistic anion) individually in the iron binding site of

the N-lobe of hTf to see how the protonation of each residue affects the coordination mode of iron (Scheme 2). Starting from a smaller model ( $sTfN^{Phys}$ ) similar to Model 2 of the physiological pH model of the N-lobe (Fig. S1), each coordinating residue is protonated, and the geometries optimized at B3LYP/6-311+G(d) level of theory (SDD for Fe atom) are depicted in Fig. S2.

The protonation of His249-N $\delta$ 1 ( $sTfN_{H249H}$ ) and Tyr95 ( $sTfN_{Y95H}$ ) resulted in the elongation of the iron-protonated residue distance: the HisN $\epsilon$ 2-iron distance elongates from 2.11 Å in  $sTfN^{Phys}$  to 2.22 Å and the Tyr95-O-iron distance elongates from 1.96 Å in  $sTfN^{Phys}$  to 2.17 Å in  $sTfN_{Y95H}$ . This elongation results in a weaker coordination of His249 and Tyr95 residues to iron in  $sTfN_{H249H}$  and  $sTfN_{Y95H}$  but still, does not affect the octahedral arrangement around iron in both complexes. However, the octahedral coordination is disrupted via the protonation of Tyr188 or the synergistic anion. The former leads to the detachment of this residue from the first coordination shell, adopting a square pyramidal coordination. The protonated Tyr188 forms hydrogen bond with O<sup>1</sup> of carbonate ( $sTfN_{Y188H}$ ). The coordination of the synergistic anion changes from bidentate to monodentate as the anion is protonated ( $sTfN_{HCO3}$ , Fig. S2).

The distance between iron and the second coordinating oxygen (O<sup>2</sup>) of bicarbonate increases to 3.21 Å, resulting in the weakening of this coordination. The loss of the coordination of one of the oxygens of bicarbonate in the equatorial plane results in a trigonal bipyramidal coordination around iron, consistent with the previously reported studies.<sup>1,2</sup>

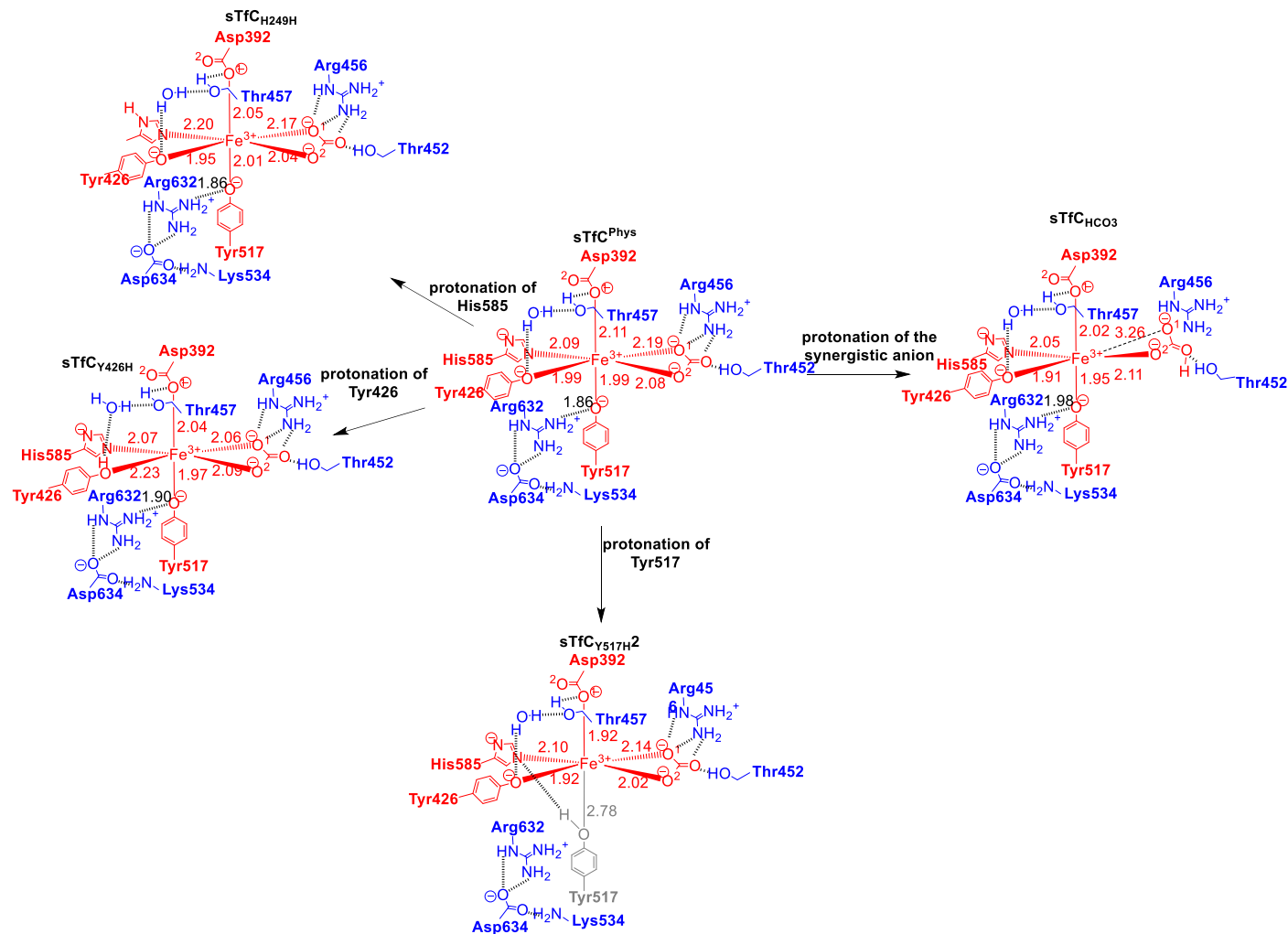
The protonation of His249 ( $sTfN_{H249H}$ ) leads to the thermodynamically stable complex with the octahedral coordination around iron. This complex is energetically followed by the complexes formed through the protonation of the synergistic carbonate ion ( $sTfN_{HCO3}$ ), the protonation of Tyr95 ( $sTfN_{Y95H}$ ) and the protonation of Tyr188 ( $sTfN_{Y188H}$ ), respectively.



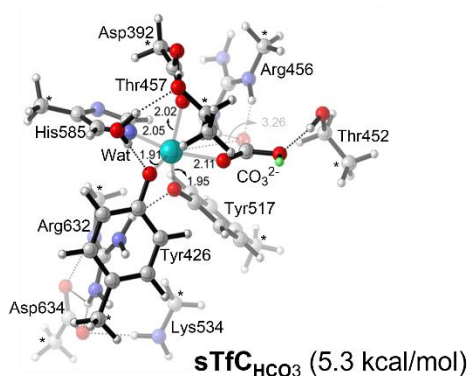
**Figure S2.** The complexes associated with the protonation of each residue in  $TfN_3^{Phys}$  and their relative free energies in parentheses. Hydrogen atom of the protonated residue is shown in green. Distances are given in Å. Atoms with asterisks (\*) are kept fixed.

For the release of iron in the C-lobe of hTf, the protonation of each residue (His585, Tyr426, Tyr517 and the synergistic anion) is also modelled individually in the iron binding site of the C-lobe of hTf (Scheme S1). Similar geometry changes in the protonated complexes of the C-lobe of hTf have been observed as in the case of the protonated complexes of the N-lobe of hTf: The octahedral arrangement is conserved for the protonation of His585 and Tyr426, and a disruption of the octahedral geometry is observed upon protonating Tyr517 and the synergistic anion (Fig. S3).

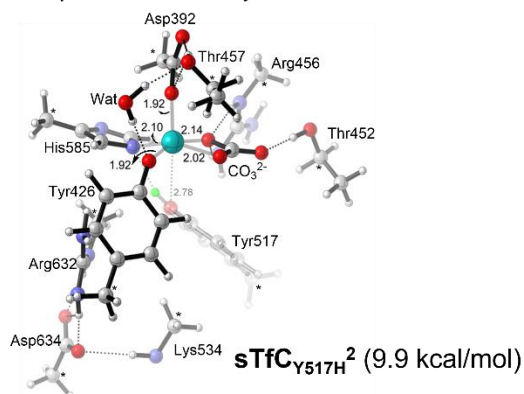
**Scheme S1.** The protonation of His585, Tyr426, Tyr517 and the synergistic anion in the physiological pH model of the C-lobe of hTf (sTfC<sup>Phys</sup>). The first and the second coordination shells are represented in red and blue respectively. The gray color of residues implies the departure of a residue from the first coordination shell. Distances are given in Å.



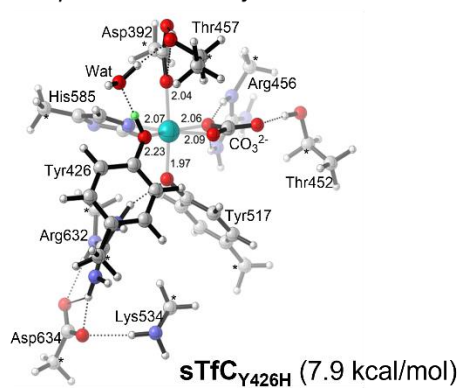
protonation of the synergistic anion



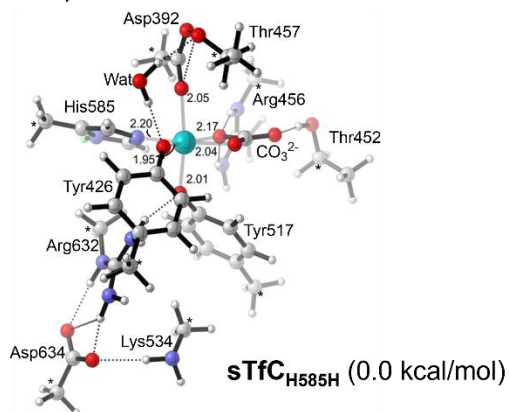
protonation of Tyr517



protonation of Tyr426



protonation of His585



**Figure S3** . The complexes associated with the protonation of each residue in the physiological pH model of the C-lobe of hTf (sTfC<sup>Phys</sup>) and their relative free energies in parentheses. Hydrogen atom of the protonated residue is shown in green. Distances are given in Å. Atoms with asterisks (\*) are kept fixed.

### 3. Coordinates

#### 3.1 N-Lobe

TfN<sup>Phys</sup>

|   |    |             |             |             |
|---|----|-------------|-------------|-------------|
| C | 0  | -1.05802500 | 3.59963700  | 1.79374900  |
| O | -1 | -0.34050600 | 2.89184800  | 0.97919700  |
| O | 0  | -1.21806300 | 4.81751800  | 1.62123600  |
| C | 0  | 5.12218300  | -1.24246600 | -1.21033300 |
| C | 0  | 4.04041200  | -0.92875600 | -2.04734900 |
| C | 0  | 5.09961800  | -0.73342200 | 0.09581800  |
| C | 0  | 2.97148500  | -0.15077000 | -1.61008900 |
| C | 0  | 4.05172800  | 0.06891700  | 0.54279400  |
| C | 0  | 2.97130500  | 0.38709300  | -0.30850500 |
| O | -1 | 2.02689700  | 1.22911100  | 0.10712800  |
| C | 0  | -5.23429000 | -0.22158900 | -4.00095800 |
| O | 0  | -5.43545500 | 1.04352600  | -1.90864900 |
| C | 0  | -4.84798100 | 3.59677600  | 0.90138500  |
| C | 0  | -5.53028000 | 2.23429000  | 1.04860800  |
| N | 0  | -4.54902300 | 1.15024300  | 0.96308200  |
| C | 0  | -4.88873900 | -0.12061300 | 0.73627700  |
| N | 0  | -3.93771800 | -0.98364300 | 0.37353400  |
| N | 0  | -6.15077800 | -0.55417600 | 0.96552000  |
| O | 0  | 1.07837000  | 5.28667500  | -0.28600800 |
| C | 0  | -2.59726400 | -3.98408900 | -1.76518400 |
| C | 0  | -2.08754600 | -2.93790700 | -2.56123100 |
| C | 0  | -2.27385900 | -3.92390900 | -0.39839500 |
| C | 0  | -1.26172200 | -1.92946500 | -2.04644000 |
| C | 0  | -1.46187600 | -2.91469000 | 0.13259200  |
| C | 0  | -0.88965300 | -1.90848300 | -0.68171500 |
| O | 0  | -0.00263100 | -1.03211900 | -0.17876600 |
| C | 0  | 1.46890500  | -4.36681100 | -2.96486400 |

TfN<sup>Acid</sup>

|   |    |             |             |             |
|---|----|-------------|-------------|-------------|
| C | 0  | -1.36617600 | 3.54384200  | 1.78398500  |
| O | -1 | -0.62614500 | 2.87594800  | 0.94695800  |
| O | 0  | -1.55851100 | 4.75624900  | 1.63647200  |
| C | 0  | 5.13305200  | -0.89196100 | -1.15409300 |
| C | 0  | 4.04288300  | -0.63920200 | -2.01306400 |
| C | 0  | 5.04120000  | -0.40354200 | 0.16189200  |
| C | 0  | 2.92792500  | 0.07919900  | -1.59702300 |
| C | 0  | 3.93352300  | 0.33456000  | 0.59028000  |
| C | 0  | 2.86427700  | 0.62635600  | -0.29113700 |
| O | -1 | 1.87973000  | 1.41771900  | 0.09611700  |
| C | 0  | -5.29531500 | -0.64177400 | -4.02461900 |
| O | 0  | -5.53631800 | 0.53575500  | -1.88756900 |
| C | 0  | -5.15921400 | 3.16888600  | 0.86486600  |
| C | 0  | -5.71852900 | 1.75287600  | 1.02920400  |
| N | 0  | -4.64820900 | 0.75451200  | 0.95123900  |
| C | 0  | -4.87675600 | -0.54685500 | 0.76765900  |
| N | 0  | -3.84644400 | -1.34506400 | 0.45570300  |
| N | 0  | -6.09888100 | -1.07383400 | 0.99675800  |
| O | 0  | 0.65438100  | 5.36827300  | -0.33823000 |
| C | 0  | -2.24165700 | -4.21681000 | -1.72033000 |
| C | 0  | -1.87371500 | -3.10692100 | -2.50883100 |
| C | 0  | -1.86085800 | -4.15724200 | -0.36935300 |
| C | 0  | -1.12767400 | -2.03140700 | -2.00376600 |
| C | 0  | -1.13037700 | -3.08356800 | 0.15124100  |
| C | 0  | -0.70458500 | -2.00345500 | -0.65545700 |
| O | 0  | 0.09450600  | -1.03703100 | -0.15205900 |
| C | 0  | 1.81649000  | -4.12950200 | -2.79728000 |



|    |    |             |             |             |    |    |             |             |             |
|----|----|-------------|-------------|-------------|----|----|-------------|-------------|-------------|
| C  | 0  | 1.86700300  | -4.17636300 | -1.49478800 | C  | 0  | 2.42212800  | -3.88364200 | -1.40550700 |
| C  | 0  | 3.37594200  | -4.24892500 | -1.25776900 | C  | 0  | 3.90690900  | -4.22837500 | -1.38015800 |
| N  | 0  | 3.72501000  | -3.91805300 | 0.14000600  | N  | 0  | 4.57573900  | -3.72848800 | -0.11690600 |
| C  | 0  | 4.86805400  | 5.05848300  | -3.33201600 | C  | 0  | 4.40340900  | 5.46520000  | -3.37726400 |
| C  | 0  | 4.80409700  | 2.73642700  | -2.27929200 | C  | 0  | 4.45599800  | 3.14720800  | -2.31165500 |
| C  | 0  | 0.95107400  | -0.24715600 | 4.61748900  | C  | 0  | 0.92737400  | -0.10273600 | 4.62657800  |
| C  | 0  | 1.10484700  | 0.10280400  | 3.28050900  | C  | 0  | 1.02367900  | 0.34096100  | 3.30960700  |
| N  | 0  | -0.36535300 | -0.57728900 | 4.84124300  | N  | 0  | -0.30549700 | -0.67646200 | 4.81200900  |
| C  | 0  | -0.95016000 | -0.41347800 | 3.63790600  | C  | 0  | -0.90489700 | -0.56396400 | 3.60845500  |
| N  | -1 | -0.11942300 | -0.02064900 | 2.65224400  | N  | -1 | -0.15286300 | 0.01372900  | 2.65409800  |
| C  | 0  | -0.26942600 | -4.73497900 | 3.78907900  | C  | 0  | 0.18464500  | -4.77717300 | 3.59248600  |
| C  | 0  | 0.36292500  | -3.42610900 | 3.30098600  | C  | 0  | 0.67576700  | -3.36675800 | 3.25694200  |
| C  | 0  | 1.26529900  | -3.62931900 | 2.09210400  | C  | 0  | 1.72298300  | -3.30586600 | 2.14307000  |
| N  | 0  | 1.73572000  | -2.34338900 | 1.48934000  | N  | 0  | 1.84062300  | -1.90333600 | 1.63285400  |
| C  | 0  | -1.85564600 | 1.24020700  | -1.55082600 | C  | 0  | -1.98722500 | 1.06115200  | -1.57266400 |
| O  | 0  | -2.09729800 | 0.91537200  | -0.27358400 | O  | 0  | -2.18931500 | 0.71483300  | -0.29058300 |
| O  | -1 | -0.56721900 | 1.46140100  | -1.72604400 | O  | -1 | -0.72153000 | 1.39981100  | -1.74155800 |
| O  | -1 | -2.77767700 | 1.30406400  | -2.42188700 | O  | -1 | -2.90841000 | 1.04076300  | -2.43711800 |
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| O  | 0  | 3.20796200  | 3.71122200  | 0.68554700  | O  | 0  | 2.88405900  | 3.98614100  | 0.66945300  |
| H  | 0  | 4.03367200  | -1.30581400 | -3.06643600 | H  | 0  | 4.08847300  | -0.99606100 | -3.03796200 |
| H  | 0  | 5.92224600  | -0.95960400 | 0.77241900  | H  | 0  | 5.86931300  | -0.56450400 | 0.85013300  |
| H  | 0  | 2.13287300  | 0.07929800  | -2.25920200 | H  | 0  | 2.09945400  | 0.27740200  | -2.26891700 |
| H  | 0  | 4.06096800  | 0.49152200  | 1.54325100  | H  | 0  | 3.90090700  | 0.74613900  | 1.59426300  |
| H  | 0  | -4.14284400 | -0.14789500 | -3.99687200 | H  | 0  | -4.22130300 | -0.43962000 | -4.07217400 |
| H  | 0  | -5.63109200 | 0.61543600  | -4.58487500 | H  | 0  | -5.81749100 | 0.15775800  | -4.56007400 |
| H  | 0  | -5.52342800 | -1.15903100 | -4.49072700 | H  | 0  | -5.49772700 | -1.59276100 | -4.53124000 |
| H  | 0  | -4.45836500 | 1.17173100  | -2.00088900 | H  | 0  | -4.58315900 | 0.76440000  | -1.99923500 |
| H  | 0  | -5.61720200 | 4.35982300  | 1.06849900  | H  | 0  | -5.99153900 | 3.86099500  | 1.03616900  |
| H  | 0  | -4.10307100 | 3.72565700  | 1.69482500  | H  | 0  | -4.42227900 | 3.36904600  | 1.65118700  |
| H  | 0  | -6.26209400 | 2.11356800  | 0.23876100  | H  | 0  | -6.43969200 | 1.56022000  | 0.22419200  |

|   |   |             |             |             |   |   |             |             |             |
|---|---|-------------|-------------|-------------|---|---|-------------|-------------|-------------|
| H | 0 | -6.04937800 | 2.17639500  | 2.01364600  | H | 0 | -6.22559700 | 1.65972500  | 1.99742500  |
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| H | 0 | -3.05398300 | -0.57407000 | 0.04537400  | H | 0 | -3.00681900 | -0.87651900 | 0.10054600  |
| H | 0 | -4.13147000 | -1.95265900 | 0.17733700  | H | 0 | -3.98139600 | -2.31689200 | 0.22375400  |
| H | 0 | -6.88445700 | 0.13356200  | 1.03710900  | H | 0 | -6.89170700 | -0.45239500 | 1.03570300  |
| H | 0 | -6.42873100 | -1.43323900 | 0.55626400  | H | 0 | -6.29433300 | -2.00388600 | 0.65973400  |
| H | 0 | 0.28863000  | 4.99061400  | 0.21112700  | H | 0 | -0.10876400 | 5.04955200  | 0.18443200  |
| H | 0 | -2.33034500 | -2.91225900 | -3.62192700 | H | 0 | -2.16782400 | -3.07955400 | -3.55610800 |
| H | 0 | -2.66047700 | -4.68719700 | 0.27563400  | H | 0 | -2.14099700 | -4.96735500 | 0.30201300  |
| H | 0 | -0.88411100 | -1.14219900 | -2.69065900 | H | 0 | -0.86141500 | -1.19854700 | -2.64635000 |
| H | 0 | -1.27129300 | -2.88616900 | 1.19831800  | H | 0 | -0.90369600 | -3.06424400 | 1.20856200  |
| H | 0 | 1.79932900  | -5.35361300 | -3.31909900 | H | 0 | 2.05286700  | -5.15008300 | -3.12577500 |
| H | 0 | 0.37486300  | -4.35920200 | -3.02435600 | H | 0 | 0.72870700  | -4.07275100 | -2.69973300 |
| H | 0 | 1.35760700  | -4.92608000 | -0.87457800 | H | 0 | 1.89474900  | -4.49792700 | -0.66831800 |
| H | 0 | 1.50893500  | -3.19422800 | -1.16812100 | H | 0 | 2.26949100  | -2.83035600 | -1.14042100 |
| H | 0 | 3.86645600  | -3.51030900 | -1.88918700 | H | 0 | 4.45001100  | -3.75435600 | -2.19700200 |
| H | 0 | 3.75842300  | -5.23648500 | -1.55961600 | H | 0 | 4.07459300  | -5.30570100 | -1.42517700 |
| H | 0 | 3.71313000  | -4.75841400 | 0.71220800  | H | 0 | 4.08691900  | -4.04133000 | 0.72618400  |
| H | 0 | 4.66907000  | -3.54670500 | 0.18561500  | H | 0 | 5.54179800  | -4.05980400 | -0.04975500 |
| H | 0 | 3.80078800  | 5.00622300  | -3.57858700 | H | 0 | 3.33707000  | 5.36847100  | -3.61369000 |
| H | 0 | 5.12153400  | 6.11328500  | -3.17662100 | H | 0 | 4.61424800  | 6.52999200  | -3.22872700 |
| H | 0 | 5.42205500  | 4.70669800  | -4.21164400 | H | 0 | 4.96395300  | 5.13240100  | -4.25990700 |
| H | 0 | 3.72628100  | 2.63351000  | -2.44345600 | H | 0 | 3.38207000  | 2.99222800  | -2.46333200 |
| H | 0 | 5.31659800  | 2.28405300  | -3.13813300 | H | 0 | 4.98093300  | 2.71637700  | -3.17401800 |
| H | 0 | 5.04203200  | 2.14566900  | -1.39076800 | H | 0 | 4.73627000  | 2.57626300  | -1.42217100 |
| H | 0 | 1.96245700  | 0.49911500  | 2.74929400  | H | 0 | 1.78341900  | 0.94177500  | 2.82345300  |
| H | 0 | -2.00752800 | -0.58297300 | 3.46237700  | H | 0 | -1.90654700 | -0.92878100 | 3.40676800  |
| H | 0 | -0.95645400 | -4.49323600 | 4.60821700  | H | 0 | -0.71386900 | -4.67782700 | 4.21165900  |
| H | 0 | -0.88521500 | -5.16315800 | 2.98532300  | H | 0 | -0.13202600 | -5.28534300 | 2.67074300  |
| H | 0 | 0.93722300  | -2.96190600 | 4.10967600  | H | 0 | 1.06565600  | -2.87495400 | 4.15356500  |
| H | 0 | -0.41905900 | -2.70388300 | 3.05881600  | H | 0 | -0.17262600 | -2.75260200 | 2.95272500  |

|   |    |             |             |             |   |    |             |             |             |
|---|----|-------------|-------------|-------------|---|----|-------------|-------------|-------------|
| H | 0  | 0.75406800  | -4.18073000 | 1.29983100  | H | 0  | 1.42856800  | -3.94024600 | 1.30488900  |
| H | 0  | 2.16107300  | -4.19119800 | 2.36316600  | H | 0  | 2.70477600  | -3.62860200 | 2.50621100  |
| H | 0  | 1.00697700  | -1.85341100 | 0.89262400  | H | 0  | 1.06107100  | -1.60696500 | 0.92513700  |
| H | 0  | 1.97446300  | -1.65996700 | 2.22107100  | H | 0  | 1.73298000  | -1.21701600 | 2.41528100  |
| H | 0  | 2.56705100  | -2.58355500 | 0.90005600  | H | 0  | 2.73451500  | -1.68007300 | 1.18998300  |
| H | 0  | 2.78129400  | 2.84965700  | 0.51296100  | H | 0  | 2.52114500  | 3.10004600  | 0.48919700  |
| H | 0  | 2.49639600  | 4.35279000  | 0.49279400  | H | 0  | 2.13884400  | 4.57782800  | 0.44296800  |
| C | -1 | 6.27016900  | -2.09980700 | -1.69349600 | C | -1 | 6.40232200  | -1.54597000 | -1.66240900 |
| H | 0  | 6.55811800  | -2.85830200 | -0.95530300 | H | 0  | 6.97199000  | -2.02121100 | -0.85596500 |
| H | 0  | 6.01923400  | -2.62018900 | -2.62299500 | H | 0  | 6.20340600  | -2.29434000 | -2.43712200 |
| H | 0  | 7.16870100  | -1.50094300 | -1.89041900 | H | 0  | 7.06775800  | -0.80135300 | -2.11475200 |
| C | -1 | -3.41522000 | -5.14682900 | -2.34616000 | C | -1 | -2.97664100 | -5.43990600 | -2.28636500 |
| H | 0  | -2.75793600 | -5.93850600 | -2.72610300 | H | 0  | -2.26729100 | -6.17192100 | -2.69102000 |
| H | 0  | -4.06273600 | -5.59205000 | -1.58445700 | H | 0  | -3.56173000 | -5.94054000 | -1.50919100 |
| H | 0  | -4.04212100 | -4.81373200 | -3.17954000 | H | 0  | -3.65294300 | -5.15529700 | -3.09831900 |
| C | -1 | -5.75803700 | -0.16794800 | -2.56610300 | C | -1 | -5.74758700 | -0.68912100 | -2.56622100 |
| H | 0  | -5.36003300 | -1.03770800 | -2.01221300 | H | 0  | -5.22582900 | -1.51874900 | -2.05512100 |
| H | 0  | -6.85283200 | -0.25632500 | -2.55499700 | H | 0  | -6.82247500 | -0.90464900 | -2.50651100 |
| C | -1 | 2.02497400  | -3.26974100 | -3.88338500 | C | -1 | 2.28017000  | -3.10982400 | -3.84142600 |
| H | 0  | 3.11507600  | -3.31357500 | -3.96724800 | H | 0  | 3.36377000  | -3.12222100 | -3.99688500 |
| H | 0  | 1.61636800  | -3.36069500 | -4.89554400 | H | 0  | 1.81525000  | -3.31584000 | -4.81029300 |
| H | 0  | 1.75715800  | -2.27955100 | -3.50025200 | H | 0  | 1.99004900  | -2.09820000 | -3.54280400 |
| C | -1 | 1.12972000  | 4.57789600  | -1.52466500 | C | -1 | 0.69456600  | 4.65554800  | -1.57541700 |
| H | 0  | 0.29110900  | 4.84783300  | -2.18265400 | H | 0  | -0.15733400 | 4.91380800  | -2.22063000 |
| H | 0  | 2.06472400  | 4.85784800  | -2.01782200 | H | 0  | 1.61777500  | 4.94516400  | -2.08443400 |
| H | 0  | 1.11667800  | 3.49122400  | -1.38047900 | H | 0  | 0.69632300  | 3.56931300  | -1.42719500 |
| C | -1 | 2.00544200  | -0.31130500 | 5.68737300  | C | -1 | 1.98402200  | -0.05383800 | 5.69395100  |
| H | 0  | 1.72397600  | 0.27780900  | 6.56876400  | H | 0  | 1.62544100  | 0.45739700  | 6.59498300  |
| H | 0  | 2.17454400  | -1.33991100 | 6.03522800  | H | 0  | 2.29290600  | -1.06112600 | 6.00296300  |
| H | 0  | 2.95897600  | 0.07674900  | 5.31431400  | H | 0  | 2.87104700  | 0.47825100  | 5.33615900  |
| C | -1 | 0.74673900  | -5.77827000 | 4.26986200  | C | -1 | 1.21313000  | -5.62634900 | 4.33954800  |

|   |    |             |             |             |
|---|----|-------------|-------------|-------------|
| H | 0  | 0.24469100  | -6.65833300 | 4.68497600  |
| H | 0  | 1.39261000  | -6.12588000 | 3.45599800  |
| H | 0  | 1.39238200  | -5.36132300 | 5.05155500  |
| C | -1 | -4.19199000 | 3.80396400  | -0.46835500 |
| H | 0  | -3.81575100 | 4.82727100  | -0.55736000 |
| H | 0  | -3.34131500 | 3.13819900  | -0.61818300 |
| H | 0  | -4.90090800 | 3.61294400  | -1.27977900 |
| C | -1 | -1.66432000 | 2.87976500  | 2.99065200  |
| H | 0  | -0.86258100 | 2.46456000  | 3.60608600  |
| H | 0  | -2.27691900 | 3.56548300  | 3.57892000  |
| H | 0  | -2.26179200 | 2.03002100  | 2.65111500  |
| C | -1 | 0.03258500  | 0.98428700  | -4.78108200 |
| H | 0  | 0.66886700  | 1.82113600  | -4.48703600 |
| H | 0  | 0.51278000  | 0.05146900  | -4.47112100 |
| H | 0  | -0.92767900 | 1.07766900  | -4.27189300 |
| H | 0  | -0.09865800 | 0.97940700  | -5.86737200 |
| C | -1 | 5.18831900  | 4.20705800  | -2.09896900 |
| H | 0  | 6.26045700  | 4.28659300  | -1.87066300 |
| H | 0  | 4.64984200  | 4.58324700  | -1.22182200 |
| C | -1 | 3.29369400  | 5.68502800  | 3.37753300  |
| H | 0  | 4.20299100  | 6.29227700  | 3.34688200  |
| H | 0  | 3.36138400  | 4.87476300  | 2.64867100  |
| H | 0  | 3.16715100  | 5.27580100  | 4.38396000  |
| H | 0  | 2.43250500  | 6.31320100  | 3.13511500  |

**TS1**

|   |    |             |             |             |
|---|----|-------------|-------------|-------------|
| C | 0  | -1.44503100 | 3.52265400  | 1.76318300  |
| O | -1 | -0.67153300 | 2.86798800  | 0.93924100  |
| O | 0  | -1.67989800 | 4.72192200  | 1.59019300  |
| C | 0  | 5.15180300  | -0.81767100 | -1.12974200 |

|   |    |             |             |             |
|---|----|-------------|-------------|-------------|
| H | 0  | 0.81003800  | -6.61222500 | 4.59175500  |
| H | 0  | 2.12001100  | -5.78721600 | 3.74381000  |
| H | 0  | 1.51349700  | -5.13773300 | 5.27289200  |
| C | -1 | -4.54035200 | 3.42911300  | -0.51395300 |
| H | 0  | -4.26007000 | 4.48210100  | -0.60971700 |
| H | 0  | -3.63611600 | 2.84085800  | -0.67247600 |
| H | 0  | -5.24039600 | 3.17427100  | -1.31566600 |
| C | -1 | -1.94727100 | 2.77083100  | 2.95743000  |
| H | 0  | -1.12966800 | 2.39481700  | 3.57832500  |
| H | 0  | -2.60579400 | 3.41096200  | 3.54662800  |
| H | 0  | -2.48864100 | 1.89279800  | 2.59691800  |
| C | -1 | -0.07678800 | 0.94189400  | -4.79032700 |
| H | 0  | 0.53288500  | 1.79321000  | -4.48133600 |
| H | 0  | 0.41480000  | 0.01869300  | -4.46894000 |
| H | 0  | -1.05098300 | 1.01455600  | -4.30550300 |
| H | 0  | -0.18214300 | 0.93462000  | -5.87899700 |
| C | -1 | 4.77107600  | 4.63626200  | -2.14240300 |
| H | 0  | 5.83965500  | 4.76582900  | -1.92195200 |
| H | 0  | 4.22221100  | 4.99222600  | -1.26337800 |
| C | -1 | 2.74432000  | 6.00533800  | 3.31505200  |
| H | 0  | 3.32618200  | 6.90116800  | 3.08082000  |
| H | 0  | 2.97694900  | 5.21348300  | 2.60056300  |
| H | 0  | 2.97803800  | 5.67957600  | 4.33279400  |
| H | 0  | 1.67888600  | 6.24163600  | 3.24845800  |
| H | 0  | 4.61307000  | -2.68481200 | -0.13027700 |

**TfN<sup>Acid</sup><sub>Y188H</sub><sup>1</sup>**

|   |    |             |             |             |
|---|----|-------------|-------------|-------------|
| C | 0  | -1.41214700 | 3.52772700  | 1.79429300  |
| O | -1 | -0.64579500 | 2.86891600  | 0.95873600  |
| O | 0  | -1.63946700 | 4.72582100  | 1.62148500  |
| C | 0  | 5.13533300  | -0.83902900 | -1.18254200 |

|   |    |             |             |             |   |    |             |             |             |
|---|----|-------------|-------------|-------------|---|----|-------------|-------------|-------------|
| C | 0  | 4.05623100  | -0.59658000 | -1.98931800 | C | 0  | 4.02470400  | -0.62736000 | -2.02427400 |
| C | 0  | 5.05592800  | -0.30990400 | 0.17927300  | C | 0  | 5.07068000  | -0.30632300 | 0.11866800  |
| C | 0  | 2.92934500  | 0.10860100  | -1.58001300 | C | 0  | 2.90684400  | 0.08408200  | -1.60186500 |
| C | 0  | 3.93882300  | 0.41624800  | 0.59865300  | C | 0  | 3.96356500  | 0.42636500  | 0.54992400  |
| C | 0  | 2.86114000  | 0.66959200  | -0.28218900 | C | 0  | 2.86553400  | 0.65440900  | -0.30906000 |
| O | -1 | 1.85888800  | 1.44515700  | 0.10187700  | O | -1 | 1.86407400  | 1.42790700  | 0.09043700  |
| C | 0  | -5.42016800 | -0.60302200 | -4.08537800 | C | 0  | -5.45832400 | -0.54713000 | -4.04200200 |
| O | 0  | -5.52884900 | 0.42763200  | -1.86618500 | O | 0  | -5.55406000 | 0.49477100  | -1.82704700 |
| C | 0  | -5.18215000 | 3.10721700  | 0.84719500  | C | 0  | -5.15377200 | 3.12738800  | 0.90547700  |
| C | 0  | -5.71808900 | 1.68472400  | 1.03242600  | C | 0  | -5.69107500 | 1.70309000  | 1.07686900  |
| N | 0  | -4.63611900 | 0.69852600  | 0.95367900  | N | 0  | -4.61225100 | 0.71415800  | 0.98507100  |
| C | 0  | -4.85262300 | -0.60802700 | 0.79112500  | C | 0  | -4.83192700 | -0.59293400 | 0.83460200  |
| N | 0  | -3.81943200 | -1.39999000 | 0.47286700  | N | 0  | -3.80132500 | -1.39161400 | 0.51553300  |
| N | 0  | -6.06436300 | -1.14488700 | 1.04763300  | N | 0  | -6.04248400 | -1.12467800 | 1.09991300  |
| O | 0  | 0.56604700  | 5.37794000  | -0.34165500 | O | 0  | 0.60738700  | 5.37423200  | -0.31880000 |
| C | 0  | -2.16931900 | -4.25952700 | -1.72140000 | C | 0  | -2.21595800 | -4.24463700 | -1.73517100 |
| C | 0  | -1.80352700 | -3.14430500 | -2.50146700 | C | 0  | -1.94941900 | -3.08419800 | -2.48573700 |
| C | 0  | -1.80232700 | -4.21166100 | -0.36689300 | C | 0  | -1.71337300 | -4.27557500 | -0.42532300 |
| C | 0  | -1.06169300 | -2.07263100 | -1.98325200 | C | 0  | -1.17337200 | -2.03130400 | -1.98272100 |
| C | 0  | -1.07886400 | -3.14106100 | 0.16793800  | C | 0  | -0.95481500 | -3.22611400 | 0.09873600  |
| C | 0  | -0.65305300 | -2.06568400 | -0.63617700 | C | 0  | -0.64784300 | -2.10675300 | -0.68677100 |
| O | 0  | 0.14986100  | -1.08856800 | -0.12622900 | O | 0  | 0.17412600  | -1.10937800 | -0.20561600 |
| C | 0  | 1.89294800  | -4.12275800 | -2.80693500 | C | 0  | 1.77720000  | -4.08443500 | -2.82995600 |
| C | 0  | 2.48341400  | -3.88253300 | -1.40849700 | C | 0  | 2.36507600  | -3.83858900 | -1.43141800 |
| C | 0  | 3.97501800  | -4.19657800 | -1.37966300 | C | 0  | 3.83685700  | -4.23385400 | -1.37496800 |
| N | 0  | 4.62580900  | -3.68349700 | -0.11357800 | N | 0  | 4.50631500  | -3.69047300 | -0.13145700 |
| C | 0  | 4.34566800  | 5.53169200  | -3.35841900 | C | 0  | 4.35195400  | 5.51011900  | -3.36834000 |
| C | 0  | 4.41223100  | 3.21217600  | -2.29638000 | C | 0  | 4.41925400  | 3.18396400  | -2.32114100 |
| C | 0  | 0.90356100  | -0.08252200 | 4.62776700  | C | 0  | 0.93303600  | -0.11004000 | 4.61587900  |
| C | 0  | 1.00224600  | 0.35426000  | 3.31102500  | C | 0  | 1.02524400  | 0.32581600  | 3.30010500  |
| N | 0  | -0.32878800 | -0.66384900 | 4.80998200  | N | 0  | -0.30677600 | -0.67730000 | 4.80761400  |

|    |    |             |             |             |
|----|----|-------------|-------------|-------------|
| C  | 0  | -0.92219800 | -0.56415800 | 3.60420100  |
| N  | -1 | -0.16608600 | 0.01378300  | 2.65022800  |
| C  | 0  | 0.23868300  | -4.74732900 | 3.61237000  |
| C  | 0  | 0.73557900  | -3.34511500 | 3.24851300  |
| C  | 0  | 1.75914400  | -3.29517500 | 2.11004000  |
| N  | 0  | 1.83110600  | -1.91513800 | 1.55034000  |
| C  | 0  | -1.98977300 | 1.02444300  | -1.58943100 |
| O  | 0  | -2.18020200 | 0.65967500  | -0.30873900 |
| O  | -1 | -0.73030500 | 1.39090400  | -1.74947300 |
| O  | -1 | -2.91053100 | 0.99905600  | -2.45564200 |
| Fe | 0  | -0.19596400 | 1.06161400  | 0.26605100  |
| O  | 0  | 2.81244000  | 4.03065700  | 0.68446800  |
| H  | 0  | 4.10660600  | -0.96571600 | -3.00935900 |
| H  | 0  | 5.88722400  | -0.44918000 | 0.86808400  |
| H  | 0  | 2.09541300  | 0.28288200  | -2.25203500 |
| H  | 0  | 3.89716100  | 0.83642400  | 1.59843300  |
| H  | 0  | -4.37292100 | -0.31583000 | -4.21962400 |
| H  | 0  | -6.04818600 | 0.18365900  | -4.51588900 |
| H  | 0  | -5.60138200 | -1.53489200 | -4.63377000 |
| H  | 0  | -4.58706800 | 0.68814300  | -1.99609400 |
| H  | 0  | -6.02330700 | 3.78748200  | 1.02265900  |
| H  | 0  | -4.43873400 | 3.32765000  | 1.62155700  |
| H  | 0  | -6.44623000 | 1.47317900  | 0.23851200  |
| H  | 0  | -6.21264900 | 1.59567200  | 2.00742100  |
| H  | 0  | -3.73138000 | 0.99548200  | 0.56808600  |
| H  | 0  | -2.98780300 | -0.92958400 | 0.10240900  |
| H  | 0  | -3.94866200 | -2.37750400 | 0.26360600  |
| H  | 0  | -6.86319700 | -0.53256300 | 1.10171300  |
| H  | 0  | -6.25618800 | -2.08199900 | 0.72878800  |
| H  | 0  | -0.20244000 | 5.05026600  | 0.16586800  |
| H  | 0  | -2.09108200 | -3.11141000 | -3.54997900 |

|    |    |             |             |             |
|----|----|-------------|-------------|-------------|
| C  | 0  | -0.90838700 | -0.57157400 | 3.60824400  |
| N  | -1 | -0.15135100 | 0.00017600  | 2.64889200  |
| C  | 0  | 0.23492900  | -4.74169800 | 3.59629700  |
| C  | 0  | 0.78490400  | -3.35867700 | 3.24612000  |
| C  | 0  | 1.89114300  | -3.34966400 | 2.18339800  |
| N  | 0  | 1.95921100  | -2.01252800 | 1.55538900  |
| C  | 0  | -2.00371400 | 1.04799700  | -1.56633700 |
| O  | 0  | -2.17360900 | 0.66864900  | -0.28669000 |
| O  | -1 | -0.74440800 | 1.40636000  | -1.73708500 |
| O  | -1 | -2.93200800 | 1.04000100  | -2.42602000 |
| Fe | 0  | -0.17913400 | 1.11655900  | 0.27555500  |
| O  | 0  | 2.85031800  | 3.99978200  | 0.67940400  |
| H  | 0  | 4.05504600  | -1.01041000 | -3.03976600 |
| H  | 0  | 5.91589700  | -0.43714700 | 0.79155200  |
| H  | 0  | 2.05979100  | 0.25113700  | -2.25911600 |
| H  | 0  | 3.93979300  | 0.86063300  | 1.54402700  |
| H  | 0  | -4.40808500 | -0.27227100 | -4.17915000 |
| H  | 0  | -6.07775100 | 0.24440800  | -4.47591700 |
| H  | 0  | -5.65076400 | -1.47953100 | -4.58565500 |
| H  | 0  | -4.61095200 | 0.74631100  | -1.96092400 |
| H  | 0  | -5.99288300 | 3.80551200  | 1.09817900  |
| H  | 0  | -4.40468100 | 3.33595000  | 1.67758400  |
| H  | 0  | -6.42230900 | 1.50030600  | 0.28379200  |
| H  | 0  | -6.18125700 | 1.60567100  | 2.05324800  |
| H  | 0  | -3.71056300 | 1.00775300  | 0.58951600  |
| H  | 0  | -2.97418500 | -0.92277400 | 0.13402400  |
| H  | 0  | -3.94517700 | -2.36382700 | 0.29109100  |
| H  | 0  | -6.84206000 | -0.51439200 | 1.16148200  |
| H  | 0  | -6.23356400 | -2.07390300 | 0.81964100  |
| H  | 0  | -0.16434200 | 5.05976600  | 0.19087700  |
| H  | 0  | -2.33888200 | -3.00103600 | -3.49734500 |

|   |    |             |             |             |   |    |             |             |             |
|---|----|-------------|-------------|-------------|---|----|-------------|-------------|-------------|
| H | 0  | -2.08577800 | -5.02835800 | 0.29436000  | H | 0  | -1.91420200 | -5.13844500 | 0.20581600  |
| H | 0  | -0.78828800 | -1.23326200 | -2.61419600 | H | 0  | -0.96354800 | -1.15664500 | -2.58817900 |
| H | 0  | -0.85544100 | -3.12755400 | 1.22539200  | H | 0  | -0.60592000 | -3.27259800 | 1.11956400  |
| H | 0  | 2.15421600  | -5.13298300 | -3.14840400 | H | 0  | 2.00438200  | -5.10965600 | -3.15093600 |
| H | 0  | 0.80341900  | -4.09188000 | -2.71811200 | H | 0  | 0.68862700  | -4.01549000 | -2.75172300 |
| H | 0  | 1.96591000  | -4.51440700 | -0.67948000 | H | 0  | 1.80471200  | -4.41627200 | -0.68994100 |
| H | 0  | 2.30875000  | -2.83656200 | -1.12890500 | H | 0  | 2.24725900  | -2.77950900 | -1.17598400 |
| H | 0  | 4.51130000  | -3.71125200 | -2.19448500 | H | 0  | 4.40499400  | -3.82569200 | -2.21080000 |
| H | 0  | 4.16548900  | -5.27008300 | -1.42471100 | H | 0  | 3.96754400  | -5.31726900 | -1.36108900 |
| H | 0  | 4.13121300  | -4.00208300 | 0.72419100  | H | 0  | 3.98435000  | -3.93325100 | 0.71547800  |
| H | 0  | 5.59610700  | -3.99951300 | -0.03530000 | H | 0  | 5.45568600  | -4.05620600 | -0.02242600 |
| H | 0  | 3.28051900  | 5.42832000  | -3.59746300 | H | 0  | 3.28450000  | 5.41154100  | -3.59916500 |
| H | 0  | 4.54919800  | 6.59761700  | -3.20784400 | H | 0  | 4.56010900  | 6.57445100  | -3.21296500 |
| H | 0  | 4.91035200  | 5.20385800  | -4.24025300 | H | 0  | 4.90806000  | 5.18594100  | -4.25691800 |
| H | 0  | 3.34000000  | 3.04924800  | -2.45202700 | H | 0  | 3.34458300  | 3.02577900  | -2.46469200 |
| H | 0  | 4.94323300  | 2.78646800  | -3.15752200 | H | 0  | 4.93798900  | 2.76284400  | -3.19194000 |
| H | 0  | 4.69370100  | 2.64211700  | -1.40676200 | H | 0  | 4.70984300  | 2.60636600  | -1.43936300 |
| H | 0  | 1.77075100  | 0.93842400  | 2.81906900  | H | 0  | 1.80566900  | 0.88317300  | 2.79666600  |
| H | 0  | -1.92091700 | -0.93474100 | 3.39857600  | H | 0  | -1.91342100 | -0.92858700 | 3.41020900  |
| H | 0  | -0.64544800 | -4.63307200 | 4.24994900  | H | 0  | -0.63956400 | -4.60737100 | 4.24356700  |
| H | 0  | -0.10309600 | -5.26177300 | 2.70280000  | H | 0  | -0.12978900 | -5.23380200 | 2.68277800  |
| H | 0  | 1.14603400  | -2.84509600 | 4.13164300  | H | 0  | 1.14283800  | -2.85348800 | 4.14864200  |
| H | 0  | -0.11641100 | -2.72815900 | 2.95896600  | H | 0  | -0.02938600 | -2.72585500 | 2.88656000  |
| H | 0  | 1.46166500  | -3.97403700 | 1.30677300  | H | 0  | 1.65770900  | -4.09288100 | 1.41006200  |
| H | 0  | 2.74909200  | -3.60164800 | 2.47331500  | H | 0  | 2.85012500  | -3.63951400 | 2.64236200  |
| H | 0  | 0.93910900  | -1.55213200 | 0.73539700  | H | 0  | 0.81365300  | -1.49466100 | 0.51069500  |
| H | 0  | 1.72626700  | -1.22770300 | 2.31652800  | H | 0  | 1.82458400  | -1.29996000 | 2.28247600  |
| H | 0  | 2.72764500  | -1.69535400 | 1.11795900  | H | 0  | 2.86829300  | -1.80024800 | 1.15282900  |
| H | 0  | 2.47020600  | 3.13747900  | 0.49977300  | H | 0  | 2.49815800  | 3.11088400  | 0.49420900  |
| H | 0  | 2.05697800  | 4.60778100  | 0.45574000  | H | 0  | 2.09933400  | 4.58591000  | 0.45993600  |
| C | -1 | 6.43199000  | -1.45511300 | -1.63274500 | C | -1 | 6.39463100  | -1.50348800 | -1.70127600 |

|   |    |             |             |             |   |    |             |             |             |
|---|----|-------------|-------------|-------------|---|----|-------------|-------------|-------------|
| H | 0  | 6.99737700  | -1.93596700 | -0.82656600 | H | 0  | 7.01444900  | -1.89708400 | -0.88825300 |
| H | 0  | 6.24635300  | -2.19570400 | -2.41803400 | H | 0  | 6.17778100  | -2.31969400 | -2.39931900 |
| H | 0  | 7.09590700  | -0.69961100 | -2.06898900 | H | 0  | 7.01587700  | -0.78504200 | -2.24896300 |
| C | -1 | -2.88782200 | -5.48125600 | -2.30156400 | C | -1 | -2.96689300 | -5.44166600 | -2.30916400 |
| H | 0  | -2.16698900 | -6.20910000 | -2.69299100 | H | 0  | -2.27291800 | -6.14161700 | -2.78970000 |
| H | 0  | -3.48538500 | -5.98645800 | -1.53701200 | H | 0  | -3.49696200 | -5.98967400 | -1.52468200 |
| H | 0  | -3.54945800 | -5.19902300 | -3.12619200 | H | 0  | -3.69434700 | -5.13170800 | -3.06547000 |
| C | -1 | -5.72409500 | -0.77010800 | -2.59758000 | C | -1 | -5.76292000 | -0.70362600 | -2.55317500 |
| H | 0  | -5.10158800 | -1.58635000 | -2.18865500 | H | 0  | -5.14941300 | -1.52527000 | -2.14117900 |
| H | 0  | -6.77177100 | -1.06399200 | -2.45235900 | H | 0  | -6.81345500 | -0.98546400 | -2.40573600 |
| C | -1 | 2.34325900  | -3.07795000 | -3.83151100 | C | -1 | 2.27186800  | -3.07682700 | -3.87238700 |
| H | 0  | 3.42787900  | -3.06596400 | -3.97888900 | H | 0  | 3.35877100  | -3.09892000 | -4.00147900 |
| H | 0  | 1.89032800  | -3.27775700 | -4.80741300 | H | 0  | 1.82893400  | -3.28652100 | -4.85085100 |
| H | 0  | 2.03056100  | -2.07714900 | -3.51968200 | H | 0  | 1.98386200  | -2.06028000 | -3.58872200 |
| C | -1 | 0.63693600  | 4.66527000  | -1.57731900 | C | -1 | 0.65599900  | 4.66842400  | -1.55934600 |
| H | 0  | -0.21680700 | 4.89729600  | -2.22971600 | H | 0  | -0.20384800 | 4.91166800  | -2.19927600 |
| H | 0  | 1.55548200  | 4.98116800  | -2.07879700 | H | 0  | 1.57088200  | 4.97899500  | -2.07042700 |
| H | 0  | 0.67052800  | 3.57965500  | -1.42821300 | H | 0  | 0.68253600  | 3.58152200  | -1.41791400 |
| C | -1 | 1.95634800  | -0.02227700 | 5.70071100  | C | -1 | 1.99775700  | -0.07244100 | 5.68004400  |
| H | 0  | 1.58868400  | 0.48125500  | 6.60258300  | H | 0  | 1.64365400  | 0.42018900  | 6.59341200  |
| H | 0  | 2.27898100  | -1.02624500 | 6.00698700  | H | 0  | 2.31684800  | -1.08328300 | 5.96734900  |
| H | 0  | 2.83714400  | 0.52257500  | 5.34654600  | H | 0  | 2.87889400  | 0.47091300  | 5.32421200  |
| C | -1 | 1.27097100  | -5.60569600 | 4.34531400  | C | -1 | 1.24972300  | -5.64154100 | 4.29924500  |
| H | 0  | 0.85987100  | -6.58406700 | 4.61387400  | H | 0  | 0.81354100  | -6.60909700 | 4.56851100  |
| H | 0  | 2.16286000  | -5.78220800 | 3.73168100  | H | 0  | 2.12118800  | -5.84018900 | 3.66390100  |
| H | 0  | 1.59769200  | -5.11376300 | 5.26814900  | H | 0  | 1.61384800  | -5.17039300 | 5.21926400  |
| C | -1 | -4.58542300 | 3.36550300  | -0.54142200 | C | -1 | -4.56847400 | 3.40986900  | -0.48396100 |
| H | 0  | -4.32674600 | 4.42256400  | -0.65121200 | H | 0  | -4.30902700 | 4.46830900  | -0.57666400 |
| H | 0  | -3.67175800 | 2.79315600  | -0.70606700 | H | 0  | -3.65744800 | 2.83850300  | -0.66749500 |
| H | 0  | -5.28955800 | 3.08867400  | -1.33223800 | H | 0  | -5.28040500 | 3.14867800  | -1.27307900 |
| C | -1 | -2.00063600 | 2.74546000  | 2.94320600  | C | -1 | -1.95849700 | 2.74655400  | 2.97377200  |



|   |    |             |             |             |
|---|----|-------------|-------------|-------------|
| H | 0  | -1.17101200 | 2.39252400  | 3.56171600  |
| H | 0  | -2.67118300 | 3.37473100  | 3.53020100  |
| H | 0  | -2.52278800 | 1.85209100  | 2.59245800  |
| C | -1 | -0.06692700 | 0.93931100  | -4.79342600 |
| H | 0  | 0.50535900  | 1.81294200  | -4.47551500 |
| H | 0  | 0.45286400  | 0.03538100  | -4.46163000 |
| H | 0  | -1.05151100 | 0.97728200  | -4.32575400 |
| H | 0  | -0.15350000 | 0.92627100  | -5.88363500 |
| C | -1 | 4.71606100  | 4.70327300  | -2.12403600 |
| H | 0  | 5.78309100  | 4.84002300  | -1.90062000 |
| H | 0  | 4.16259000  | 5.05437800  | -1.24579200 |
| C | -1 | 2.64294800  | 6.04593500  | 3.32252300  |
| H | 0  | 3.26835900  | 6.92437900  | 3.14033800  |
| H | 0  | 2.89255300  | 5.25654800  | 2.61120000  |
| H | 0  | 2.80106400  | 5.69718200  | 4.34712600  |
| H | 0  | 1.59235200  | 6.32029300  | 3.19437700  |
| H | 0  | 4.64474000  | -2.64064400 | -0.12908700 |

**TfN<sup>Acid</sup><sub>Y188H<sup>2</sup></sub>**

|   |    |             |             |             |
|---|----|-------------|-------------|-------------|
| C | 0  | -1.17761200 | 3.44591300  | 1.99059000  |
| O | -1 | -0.44502000 | 2.80133900  | 1.10828000  |
| O | 0  | -1.40126900 | 4.64697100  | 1.85397500  |
| C | 0  | 5.11205900  | -0.90857800 | -1.55533400 |
| C | 0  | 3.94061500  | -0.68407000 | -2.30111300 |
| C | 0  | 5.18404600  | -0.33826200 | -0.27086000 |
| C | 0  | 2.86068200  | 0.02651700  | -1.77758500 |
| C | 0  | 4.12256000  | 0.38812700  | 0.25857600  |
| C | 0  | 2.93332000  | 0.56817100  | -0.48004200 |
| O | -1 | 1.94392500  | 1.28051400  | 0.05457500  |
| C | 0  | -5.61239100 | -0.08735900 | -3.85074700 |
| O | 0  | -5.59852300 | 0.85794100  | -1.58819100 |

|   |    |             |             |             |
|---|----|-------------|-------------|-------------|
| H | 0  | -1.12366700 | 2.38256300  | 3.57873000  |
| H | 0  | -2.61714500 | 3.37727000  | 3.57216400  |
| H | 0  | -2.49059000 | 1.85947200  | 2.62213300  |
| C | -1 | -0.10917100 | 0.96787200  | -4.79079400 |
| H | 0  | 0.50314800  | 1.81605600  | -4.47859100 |
| H | 0  | 0.37112600  | 0.04274700  | -4.45786800 |
| H | 0  | -1.08920000 | 1.05033200  | -4.31930200 |
| H | 0  | -0.20107500 | 0.95530000  | -5.88048900 |
| C | -1 | 4.73025200  | 4.67282000  | -2.14233700 |
| H | 0  | 5.79974700  | 4.80421300  | -1.92789300 |
| H | 0  | 4.18619300  | 5.02084700  | -1.25706000 |
| C | -1 | 2.71804800  | 6.00294500  | 3.33014500  |
| H | 0  | 3.39771700  | 6.84711700  | 3.18383000  |
| H | 0  | 2.94488700  | 5.21264200  | 2.61229400  |
| H | 0  | 2.82424500  | 5.62772000  | 4.35204400  |
| H | 0  | 1.68914900  | 6.33932900  | 3.17634100  |
| H | 0  | 4.58088900  | -2.65278900 | -0.19869300 |

**TS2**

|   |    |             |             |             |
|---|----|-------------|-------------|-------------|
| C | 0  | 1.15115200  | -3.45440500 | 1.98723100  |
| O | -1 | 0.42194100  | -2.80378400 | 1.10660900  |
| O | 0  | 1.36683200  | -4.65668400 | 1.84905900  |
| C | 0  | -5.11360500 | 0.94547000  | -1.54833600 |
| C | 0  | -3.94622400 | 0.71039700  | -2.29671300 |
| C | 0  | -5.18693300 | 0.37824600  | -0.26347900 |
| C | 0  | -2.87044000 | -0.00701200 | -1.77499600 |
| C | 0  | -4.12902200 | -0.35567300 | 0.26523900  |
| C | 0  | -2.94358300 | -0.54532700 | -0.47625900 |
| O | -1 | -1.95700000 | -1.26471300 | 0.05677000  |
| C | 0  | 5.60625500  | 0.05109900  | -3.85578000 |
| O | 0  | 5.58680600  | -0.89591900 | -1.59395900 |

|   |    |             |             |             |   |    |             |             |             |
|---|----|-------------|-------------|-------------|---|----|-------------|-------------|-------------|
| C | 0  | -4.97679000 | 3.38710500  | 1.26396000  | C | 0  | 4.95305500  | -3.42666400 | 1.25600200  |
| C | 0  | -5.61447600 | 2.00474200  | 1.41784900  | C | 0  | 5.60210600  | -2.04986500 | 1.41120700  |
| N | 0  | -4.61430300 | 0.94700800  | 1.23624800  | N | 0  | 4.60974600  | -0.98431000 | 1.23234600  |
| C | 0  | -4.94307000 | -0.32065300 | 0.97603200  | C | 0  | 4.94797500  | 0.28057400  | 0.97075200  |
| N | 0  | -3.99394200 | -1.14786100 | 0.52029800  | N | 0  | 4.00376100  | 1.11521800  | 0.51854600  |
| N | 0  | -6.17173400 | -0.79054100 | 1.26424300  | N | 0  | 6.18120800  | 0.74082700  | 1.25523600  |
| O | 0  | 0.83906600  | 5.30807700  | -0.08879400 | O | 0  | -0.88251800 | -5.29863600 | -0.09047400 |
| C | 0  | -2.60841400 | -4.05095000 | -1.77292600 | C | 0  | 2.63588100  | 4.03301000  | -1.77084600 |
| C | 0  | -2.13806000 | -2.91202900 | -2.45284500 | C | 0  | 2.14714500  | 2.90310200  | -2.45293000 |
| C | 0  | -2.31200500 | -4.12280500 | -0.40025600 | C | 0  | 2.35456100  | 4.09920200  | -0.39490500 |
| C | 0  | -1.35121500 | -1.93765100 | -1.82600300 | C | 0  | 1.35613200  | 1.93331800  | -1.82433700 |
| C | 0  | -1.53997900 | -3.14935700 | 0.24934100  | C | 0  | 1.57839100  | 3.13008200  | 0.25599300  |
| C | 0  | -1.02027700 | -2.06783000 | -0.47331400 | C | 0  | 1.03883400  | 2.05949800  | -0.46814500 |
| O | 0  | -0.14484300 | -1.15861900 | 0.09587900  | O | 0  | 0.15654800  | 1.15833600  | 0.10431800  |
| C | 0  | 1.26242200  | -3.93542700 | -3.13856500 | C | 0  | -1.24250900 | 3.95346400  | -3.13540400 |
| C | 0  | 1.63809500  | -3.61478200 | -1.67858800 | C | 0  | -1.60843700 | 3.63035800  | -1.67344900 |
| C | 0  | 2.98719200  | -4.22317500 | -1.27438600 | C | 0  | -2.95025700 | 4.24335600  | -1.25015500 |
| N | 0  | 3.75250200  | -3.33906400 | -0.33870900 | N | 0  | -3.69629500 | 3.36886300  | -0.29703500 |
| C | 0  | 4.52708300  | 5.61340400  | -3.09929800 | C | 0  | -4.57594100 | -5.57690500 | -3.09726300 |
| C | 0  | 4.52879300  | 3.09958300  | -2.65749500 | C | 0  | -4.55571500 | -3.06340200 | -2.65425500 |
| C | 0  | 1.15132900  | -0.53079900 | 4.49016600  | C | 0  | -1.15054900 | 0.54331100  | 4.48928500  |
| C | 0  | 1.16574000  | 0.08176900  | 3.24613200  | C | 0  | -1.17026800 | -0.06865700 | 3.24473100  |
| N | 0  | -0.05229700 | -1.18610200 | 4.65362500  | N | 0  | 0.05902900  | 1.18666100  | 4.65420000  |
| C | 0  | -0.71854300 | -0.93867900 | 3.51888300  | C | 0  | 0.72446200  | 0.93195200  | 3.52073000  |
| N | -1 | -0.04102200 | -0.17967800 | 2.61849500  | N | -1 | 0.04128900  | 0.17881600  | 2.61976200  |
| C | 0  | 0.90667700  | -5.44253600 | 2.48009600  | C | 0  | -0.88063700 | 5.46401700  | 2.47924900  |
| C | 0  | 1.16492000  | -3.93823600 | 2.35528700  | C | 0  | -1.10761100 | 3.95504200  | 2.34343100  |
| C | 0  | 2.56786000  | -3.51525400 | 2.80579000  | C | 0  | -2.50006900 | 3.49885000  | 2.79518800  |
| N | 0  | 2.99418200  | -2.33942300 | 2.01795200  | N | 0  | -2.92783500 | 2.34965900  | 1.95973400  |
| C | 0  | -2.02404600 | 1.21850000  | -1.43391400 | C | 0  | 2.01055500  | -1.23071300 | -1.43538800 |
| O | 0  | -2.17262500 | 0.83955100  | -0.16606600 | O | 0  | 2.16337500  | -0.85607800 | -0.16727800 |

|    |    |             |             |             |    |    |             |             |             |
|----|----|-------------|-------------|-------------|----|----|-------------|-------------|-------------|
| O  | -1 | -0.73423700 | 1.49953500  | -1.65526300 | O  | -1 | 0.71765200  | -1.50178000 | -1.65615300 |
| O  | -1 | -2.96498900 | 1.28636000  | -2.26671300 | O  | -1 | 2.94923700  | -1.30433500 | -2.26984000 |
| Fe | 0  | -0.06542700 | 1.18288800  | 0.21435300  | Fe | 0  | 0.05049000  | -1.18662600 | 0.20860800  |
| O  | 0  | 3.02838100  | 3.77799600  | 0.77900200  | O  | 0  | -3.05836400 | -3.75248500 | 0.78316900  |
| H  | 0  | 3.86656300  | -1.09297200 | -3.30375200 | H  | 0  | -3.87061600 | 1.11847700  | -3.29954200 |
| H  | 0  | 6.08112300  | -0.48339000 | 0.32677100  | H  | 0  | -6.08192900 | 0.53010500  | 0.33567900  |
| H  | 0  | 1.95639800  | 0.18582200  | -2.35711800 | H  | 0  | -1.96861200 | -0.17397700 | -2.35624200 |
| H  | 0  | 4.18399500  | 0.83127100  | 1.24732500  | H  | 0  | -4.19329900 | -0.80080400 | 1.25313800  |
| H  | 0  | -4.55054900 | 0.12652600  | -4.00556700 | H  | 0  | 4.54305600  | -0.15592300 | -4.01058400 |
| H  | 0  | -6.19111900 | 0.75995300  | -4.23205400 | H  | 0  | 6.17955200  | -0.79953200 | -4.23790300 |
| H  | 0  | -5.87743900 | -0.98024100 | -4.42886600 | H  | 0  | 5.87679200  | 0.94275900  | -4.43321200 |
| H  | 0  | -4.65112300 | 1.07145600  | -1.74760100 | H  | 0  | 4.63788200  | -1.10276200 | -1.75296500 |
| H  | 0  | -5.75980100 | 4.12448800  | 1.47304700  | H  | 0  | 5.73070600  | -4.17100400 | 1.46027400  |
| H  | 0  | -4.20394700 | 3.52909400  | 2.02810500  | H  | 0  | 4.18159200  | -3.56437300 | 2.02234700  |
| H  | 0  | -6.39299300 | 1.88531200  | 0.65331900  | H  | 0  | 6.38030000  | -1.93547500 | 0.64555800  |
| H  | 0  | -6.06821000 | 1.90662500  | 2.41162600  | H  | 0  | 6.05815000  | -1.95652900 | 2.40438000  |
| H  | 0  | -3.70778000 | 1.20689200  | 0.83441800  | H  | 0  | 3.70060300  | -1.23726400 | 0.83220700  |
| H  | 0  | -3.15775300 | -0.70201000 | 0.13436300  | H  | 0  | 3.16361600  | 0.67544100  | 0.13409500  |
| H  | 0  | -4.20405100 | -2.09474800 | 0.24592600  | H  | 0  | 4.22137300  | 2.05932200  | 0.24027400  |
| H  | 0  | -6.91320800 | -0.14123100 | 1.47309000  | H  | 0  | 6.91888700  | 0.08505000  | 1.45741000  |
| H  | 0  | -6.45667000 | -1.68450900 | 0.89637400  | H  | 0  | 6.47139700  | 1.63238600  | 0.88553400  |
| H  | 0  | 0.05852400  | 5.00158000  | 0.41094000  | H  | 0  | -0.09800000 | -4.99998300 | 0.40773700  |
| H  | 0  | -2.36893300 | -2.78652300 | -3.50760900 | H  | 0  | 2.36656000  | 2.78165300  | -3.51058900 |
| H  | 0  | -2.67542900 | -4.96612700 | 0.18228700  | H  | 0  | 2.73342300  | 4.93447400  | 0.18938000  |
| H  | 0  | -0.97981700 | -1.08206500 | -2.37989000 | H  | 0  | 0.97041600  | 1.08483000  | -2.37939600 |
| H  | 0  | -1.33571800 | -3.23695500 | 1.31067300  | H  | 0  | 1.38807700  | 3.21226900  | 1.32023200  |
| H  | 0  | 1.50499200  | -4.98376700 | -3.35944400 | H  | 0  | -1.48844700 | 5.00175500  | -3.35329100 |
| H  | 0  | 0.17898200  | -3.84486400 | -3.24229700 | H  | 0  | -0.15966300 | 3.86464400  | -3.24902600 |
| H  | 0  | 0.86196700  | -3.98564400 | -1.00493900 | H  | 0  | -0.82176200 | 3.99178300  | -1.00642400 |
| H  | 0  | 1.66609400  | -2.52791600 | -1.54332600 | H  | 0  | -1.64347300 | 2.54307000  | -1.54267300 |
| H  | 0  | 3.62833400  | -4.37778500 | -2.14777600 | H  | 0  | -3.59488000 | 4.40379400  | -2.12179400 |

|   |    |             |             |             |   |    |             |             |             |
|---|----|-------------|-------------|-------------|---|----|-------------|-------------|-------------|
| H | 0  | 2.85637600  | -5.18985000 | -0.78259200 | H | 0  | -2.80317700 | 5.21400200  | -0.76922200 |
| H | 0  | 4.61011400  | -3.80146600 | -0.03281300 | H | 0  | -4.55013100 | 3.83872600  | 0.00675500  |
| H | 0  | 4.04617600  | -2.48530800 | -0.83596000 | H | 0  | -4.00534500 | 2.52778500  | -0.79752200 |
| H | 0  | 3.45524600  | 5.60406400  | -3.33087000 | H | 0  | -3.50420500 | -5.57658800 | -3.32951900 |
| H | 0  | 4.76815500  | 6.59997500  | -2.68865400 | H | 0  | -4.82515900 | -6.56156500 | -2.68688400 |
| H | 0  | 5.06541800  | 5.50435600  | -4.04910600 | H | 0  | -5.11390800 | -5.46282700 | -4.04667200 |
| H | 0  | 3.44733400  | 3.01403200  | -2.81713800 | H | 0  | -3.47356300 | -2.98686100 | -2.81372300 |
| H | 0  | 5.02340300  | 2.89186800  | -3.61498500 | H | 0  | -5.04833900 | -2.85137900 | -3.61180300 |
| H | 0  | 4.81255400  | 2.31362500  | -1.95126700 | H | 0  | -4.83318400 | -2.27515900 | -1.94813300 |
| H | 0  | 1.91138300  | 0.71203100  | 2.77776300  | H | 0  | -1.91940200 | -0.69576200 | 2.77745100  |
| H | 0  | -1.71757000 | -1.31014200 | 3.31503300  | H | 0  | 1.72730700  | 1.29361300  | 3.31815300  |
| H | 0  | -0.11657100 | -5.65736500 | 2.14761700  | H | 0  | 0.13154300  | 5.70115000  | 2.12922900  |
| H | 0  | 1.57299200  | -5.97781200 | 1.78806200  | H | 0  | -1.57037100 | 5.99018300  | 1.80381800  |
| H | 0  | 0.42820600  | -3.37151700 | 2.93730500  | H | 0  | -0.35831800 | 3.39938500  | 2.91951400  |
| H | 0  | 1.03506600  | -3.63961200 | 1.30835500  | H | 0  | -0.97326200 | 3.67085900  | 1.29352200  |
| H | 0  | 3.29041400  | -4.31949200 | 2.61110100  | H | 0  | -3.23865000 | 4.29591300  | 2.64471700  |
| H | 0  | 2.58517900  | -3.31511300 | 3.88302000  | H | 0  | -2.50515900 | 3.23288700  | 3.85580300  |
| H | 0  | -0.16422200 | -1.12364500 | 1.10077100  | H | 0  | 0.19137200  | 1.10930100  | 1.10885900  |
| H | 0  | 2.30933000  | -1.58646800 | 2.13267900  | H | 0  | -2.23004300 | 1.60004700  | 2.01430800  |
| H | 0  | 3.86837200  | -1.95789500 | 2.37782200  | H | 0  | -3.79102200 | 1.93609500  | 2.31258600  |
| H | 0  | 2.62744900  | 2.92074500  | 0.55239300  | H | 0  | -2.65212700 | -2.89856100 | 0.55352600  |
| H | 0  | 2.30402200  | 4.41510400  | 0.62033200  | H | 0  | -2.33943300 | -4.39506900 | 0.62189700  |
| C | -1 | 6.22921400  | -1.78079300 | -2.08828600 | C | -1 | -6.22218900 | 1.82952900  | -2.07887600 |
| H | 0  | 6.77381500  | -2.27410900 | -1.27684200 | H | 0  | -6.77613600 | 2.30721100  | -1.26466200 |
| H | 0  | 5.84533500  | -2.55342800 | -2.76301000 | H | 0  | -5.82722500 | 2.61577300  | -2.73098400 |
| H | 0  | 6.96361700  | -1.19754200 | -2.65720000 | H | 0  | -6.94883300 | 1.25925400  | -2.67059100 |
| C | -1 | -3.35192500 | -5.17940400 | -2.49646300 | C | -1 | 3.38299900  | 5.15863300  | -2.49458300 |
| H | 0  | -2.64004500 | -5.90677000 | -2.90338600 | H | 0  | 2.67376400  | 5.89350200  | -2.89251300 |
| H | 0  | -4.02041100 | -5.71363000 | -1.81541500 | H | 0  | 4.06097700  | 5.68419800  | -1.81618300 |
| H | 0  | -3.94250900 | -4.79127900 | -3.33130800 | H | 0  | 3.96396700  | 4.76988900  | -3.33588200 |
| C | -1 | -5.89017000 | -0.29372100 | -2.36301700 | C | -1 | 5.88574200  | 0.25448700  | -2.36798800 |

|   |    |             |             |             |   |    |             |             |             |
|---|----|-------------|-------------|-------------|---|----|-------------|-------------|-------------|
| H | 0  | -5.31354600 | -1.16470500 | -2.00262400 | H | 0  | 5.31500200  | 1.12893400  | -2.00672100 |
| H | 0  | -6.95105900 | -0.52312900 | -2.20066300 | H | 0  | 6.94816300  | 0.47676600  | -2.20573200 |
| C | -1 | 1.94101400  | -3.01051700 | -4.15826000 | C | -1 | -1.92738100 | 3.02975000  | -4.15246300 |
| H | 0  | 3.03348200  | -3.07342900 | -4.09999700 | H | 0  | -3.01930000 | 3.09194600  | -4.08543500 |
| H | 0  | 1.65197600  | -3.27171900 | -5.18092000 | H | 0  | -1.64585300 | 3.29208800  | -5.17706300 |
| H | 0  | 1.65435100  | -1.96847600 | -3.98149200 | H | 0  | -1.63948600 | 1.98736100  | -3.97898900 |
| C | -1 | 0.84995300  | 4.66759100  | -1.36416000 | C | -1 | -0.88925100 | -4.65846200 | -1.36599200 |
| H | 0  | -0.05116800 | 4.90279100  | -1.94647500 | H | 0  | 0.00680800  | -4.90552800 | -1.95122600 |
| H | 0  | 1.72434700  | 5.04024200  | -1.90320500 | H | 0  | -1.77021000 | -5.01977900 | -1.90204200 |
| H | 0  | 0.93071100  | 3.57660200  | -1.28378100 | H | 0  | -0.95558500 | -3.56656900 | -1.28580500 |
| C | -1 | 2.22298200  | -0.53530900 | 5.54457100  | C | -1 | -2.21691100 | 0.54844300  | 5.54858700  |
| H | 0  | 1.87677500  | -0.06896500 | 6.47468000  | H | 0  | -1.86977100 | 0.06929200  | 6.47174800  |
| H | 0  | 2.53511500  | -1.55653500 | 5.79743000  | H | 0  | -2.51788100 | 1.56967200  | 5.81485600  |
| H | 0  | 3.10533200  | 0.01469500  | 5.20242000  | H | 0  | -3.10645400 | 0.00991000  | 5.20670000  |
| C | -1 | 1.11346500  | -5.97125800 | 3.90082800  | C | -1 | -1.06961000 | 5.97756000  | 3.90820500  |
| H | 0  | 0.88178500  | -7.03923900 | 3.96735300  | H | 0  | -0.86481600 | 7.05073700  | 3.97629900  |
| H | 0  | 2.14842600  | -5.83772900 | 4.23286700  | H | 0  | -2.09329400 | 5.81500100  | 4.26234500  |
| H | 0  | 0.46923600  | -5.44176000 | 4.61188500  | H | 0  | -0.39610400 | 5.46075700  | 4.60114900  |
| C | -1 | -4.38765600 | 3.62827200  | -0.13025000 | C | -1 | 4.35711400  | -3.65835200 | -0.13688600 |
| H | 0  | -4.07248300 | 4.67034800  | -0.23450000 | H | 0  | 4.03343900  | -4.69760200 | -0.24365500 |
| H | 0  | -3.50817900 | 3.01024200  | -0.31382900 | H | 0  | 3.48163400  | -3.03307900 | -0.31498800 |
| H | 0  | -5.11793000 | 3.40032700  | -0.91261400 | H | 0  | 5.08625400  | -3.43341500 | -0.92114200 |
| C | -1 | -1.67926300 | 2.63559100  | 3.16929200  | C | -1 | 1.65957800  | -2.64877300 | 3.16642000  |
| H | 0  | -0.82290000 | 2.22930000  | 3.71445000  | H | 0  | 0.80691800  | -2.23491300 | 3.71156300  |
| H | 0  | -2.28974500 | 3.26008100  | 3.82215400  | H | 0  | 2.26458900  | -3.27868200 | 3.81917400  |
| H | 0  | -2.25060900 | 1.77518700  | 2.81207700  | H | 0  | 2.23884700  | -1.79368000 | 2.80911700  |
| C | -1 | -0.24912400 | 1.19965300  | -4.75308600 | C | -1 | 0.23139800  | -1.19574900 | -4.75319500 |
| H | 0  | 0.41496200  | 2.01147400  | -4.44956000 | H | 0  | -0.43655900 | -2.00493100 | -4.45107800 |
| H | 0  | 0.20592500  | 0.24562300  | -4.46959600 | H | 0  | -0.21916100 | -0.24002900 | -4.46821400 |
| H | 0  | -1.20018200 | 1.30845700  | -4.23054400 | H | 0  | 1.18199300  | -1.30980300 | -4.23092200 |
| H | 0  | -0.39439100 | 1.22326100  | -5.83659100 | H | 0  | 0.37652900  | -1.21829000 | -5.83673700 |

|   |    |            |             |             |
|---|----|------------|-------------|-------------|
| C | -1 | 4.89105500 | 4.48967000  | -2.12388300 |
| H | 0  | 5.96750800 | 4.53105100  | -1.90805900 |
| H | 0  | 4.37378800 | 4.62967100  | -1.16729800 |
| C | -1 | 3.18019900 | 5.61565700  | 3.49496800  |
| H | 0  | 4.09072800 | 6.22129500  | 3.48005600  |
| H | 0  | 3.25318600 | 4.81520500  | 2.75730300  |
| H | 0  | 3.04316000 | 5.19731100  | 4.49634400  |
| H | 0  | 2.32353700 | 6.25000500  | 3.25186700  |
| H | 0  | 3.26771100 | -2.93686700 | 0.58927600  |

|   |    |             |             |             |
|---|----|-------------|-------------|-------------|
| C | -1 | -4.92976700 | -4.45047900 | -2.12118600 |
| H | 0  | -6.00645300 | -4.48266600 | -1.90497400 |
| H | 0  | -4.41348100 | -4.59574300 | -1.16484900 |
| C | -1 | -3.22110200 | -5.59365200 | 3.49486100  |
| H | 0  | -4.13483700 | -6.19430200 | 3.47574200  |
| H | 0  | -3.28787600 | -4.79075200 | 2.75928800  |
| H | 0  | -3.08450000 | -5.17903400 | 4.49785800  |
| H | 0  | -2.36727600 | -6.23197800 | 3.25221800  |
| H | 0  | -3.19200100 | 2.87693800  | 0.73013400  |

**TfN<sup>Acid</sup><sub>K296H</sub>**

|   |    |             |             |             |
|---|----|-------------|-------------|-------------|
| C | 0  | -1.22145100 | 3.42450600  | 2.00212300  |
| O | -1 | -0.48582600 | 2.79249300  | 1.11407800  |
| O | 0  | -1.46239100 | 4.62292600  | 1.87231000  |
| C | 0  | 5.10139600  | -0.84649000 | -1.58423800 |
| C | 0  | 3.92731500  | -0.62869100 | -2.32480800 |
| C | 0  | 5.17028900  | -0.29073800 | -0.29527700 |
| C | 0  | 2.84347800  | 0.06790300  | -1.79580400 |
| C | 0  | 4.10088200  | 0.42105800  | 0.24447500  |
| C | 0  | 2.91328000  | 0.59943100  | -0.49475000 |
| O | -1 | 1.91710800  | 1.30755600  | 0.04120500  |
| C | 0  | -5.63556900 | -0.15596300 | -3.82217900 |
| O | 0  | -5.62860700 | 0.78844600  | -1.55894800 |
| C | 0  | -5.01520100 | 3.30615000  | 1.30076100  |
| C | 0  | -5.63354800 | 1.91434900  | 1.44952300  |
| N | 0  | -4.62186200 | 0.87046100  | 1.25244000  |
| C | 0  | -4.93626400 | -0.39919000 | 0.98488100  |
| N | 0  | -3.97731700 | -1.21377800 | 0.52483700  |
| N | 0  | -6.15875400 | -0.88562600 | 1.27281100  |
| O | 0  | 0.76480000  | 5.31566900  | -0.08040900 |
| C | 0  | -2.55857900 | -4.08365900 | -1.78483000 |

|    |    |             |             |             |
|----|----|-------------|-------------|-------------|
| C  | 0  | -2.09568000 | -2.94531600 | -2.47123300 |
| C  | 0  | -2.25299700 | -4.15172900 | -0.41439500 |
| C  | 0  | -1.31405800 | -1.96277300 | -1.85064400 |
| C  | 0  | -1.48420100 | -3.17136100 | 0.22797900  |
| C  | 0  | -0.98001600 | -2.08583600 | -0.49864500 |
| O  | 0  | -0.12235000 | -1.15856700 | 0.07257500  |
| C  | 0  | 1.35433300  | -3.93295400 | -3.14599000 |
| C  | 0  | 1.77049900  | -3.60122600 | -1.70085400 |
| C  | 0  | 3.15474500  | -4.14962900 | -1.33921300 |
| N  | 0  | 3.77866100  | -3.38977500 | -0.22919100 |
| C  | 0  | 4.41908500  | 5.65838500  | -3.14323200 |
| C  | 0  | 4.47582400  | 3.15513100  | -2.65025100 |
| C  | 0  | 1.18505200  | -0.54116000 | 4.46940400  |
| C  | 0  | 1.17897300  | 0.08763100  | 3.22833400  |
| N  | 0  | 0.00163100  | -1.22495800 | 4.63213300  |
| C  | 0  | -0.68154900 | -0.97198400 | 3.50580800  |
| N  | -1 | -0.03219800 | -0.18742300 | 2.61233600  |
| C  | 0  | 1.02985300  | -5.40364100 | 2.45681500  |
| C  | 0  | 1.23595600  | -3.88693600 | 2.37083300  |
| C  | 0  | 2.61456100  | -3.44161600 | 2.86464400  |
| N  | 0  | 3.00690200  | -2.19011800 | 2.14299500  |
| C  | 0  | -2.05927300 | 1.19256700  | -1.42373100 |
| O  | 0  | -2.19179000 | 0.80370800  | -0.15831900 |
| O  | -1 | -0.77407500 | 1.49544600  | -1.65179700 |
| O  | -1 | -3.00539000 | 1.25384300  | -2.25048600 |
| Fe | 0  | -0.07911100 | 1.19369400  | 0.19403700  |
| O  | 0  | 2.98328200  | 3.81271000  | 0.76908800  |
| H  | 0  | 3.85426000  | -1.03187100 | -3.32949800 |
| H  | 0  | 6.07224300  | -0.42877000 | 0.29714700  |
| H  | 0  | 1.93676200  | 0.22346600  | -2.37253100 |
| H  | 0  | 4.16441900  | 0.86762200  | 1.23224300  |

|   |   |             |             |             |
|---|---|-------------|-------------|-------------|
| H | 0 | -4.57602600 | 0.06782700  | -3.97855700 |
| H | 0 | -6.22286100 | 0.68595600  | -4.20232100 |
| H | 0 | -5.89305100 | -1.05114400 | -4.40008900 |
| H | 0 | -4.68541000 | 1.01555900  | -1.72403600 |
| H | 0 | -5.80509400 | 4.03116400  | 1.52665500  |
| H | 0 | -4.23509700 | 3.45137100  | 2.05684100  |
| H | 0 | -6.41647200 | 1.79128300  | 0.69009200  |
| H | 0 | -6.07837100 | 1.80279000  | 2.44589700  |
| H | 0 | -3.72104100 | 1.14440600  | 0.84640300  |
| H | 0 | -3.14957400 | -0.75434800 | 0.13597600  |
| H | 0 | -4.18317700 | -2.15584400 | 0.23070400  |
| H | 0 | -6.90941800 | -0.24450700 | 1.47463200  |
| H | 0 | -6.43191300 | -1.78141100 | 0.90012000  |
| H | 0 | -0.00769700 | 4.99799500  | 0.42460100  |
| H | 0 | -2.33103400 | -2.82537100 | -3.52558500 |
| H | 0 | -2.60763500 | -4.99607400 | 0.17207300  |
| H | 0 | -0.95299000 | -1.10461600 | -2.40739100 |
| H | 0 | -1.27668300 | -3.25453900 | 1.28921200  |
| H | 0 | 1.64522400  | -4.96545400 | -3.38524700 |
| H | 0 | 0.26406000  | -3.89909700 | -3.21616200 |
| H | 0 | 1.03263800  | -4.00152200 | -0.99804200 |
| H | 0 | 1.76459500  | -2.51436600 | -1.56203600 |
| H | 0 | 3.80783300  | -4.13357500 | -2.22397900 |
| H | 0 | 3.06917200  | -5.19797600 | -1.03362100 |
| H | 0 | 4.58528200  | -3.90762400 | 0.11742100  |
| H | 0 | 4.16434500  | -2.53384100 | -0.62798500 |
| H | 0 | 3.34783800  | 5.62009900  | -3.37482300 |
| H | 0 | 4.63783800  | 6.65848100  | -2.75325000 |
| H | 0 | 4.96029100  | 5.54158200  | -4.09045100 |
| H | 0 | 3.39657700  | 3.04244800  | -2.80760300 |
| H | 0 | 4.97459100  | 2.93955000  | -3.60378200 |



|   |    |             |             |             |
|---|----|-------------|-------------|-------------|
| H | 0  | 4.77678000  | 2.38906100  | -1.92955300 |
| H | 0  | 1.88701200  | 0.77538600  | 2.78121900  |
| H | 0  | -1.67224100 | -1.36649600 | 3.30546300  |
| H | 0  | 0.02409000  | -5.63661300 | 2.08756500  |
| H | 0  | 1.73151400  | -5.89552200 | 1.76943000  |
| H | 0  | 0.47438400  | -3.35702500 | 2.95387900  |
| H | 0  | 1.12163400  | -3.57804600 | 1.32597200  |
| H | 0  | 3.38281500  | -4.18272300 | 2.62861700  |
| H | 0  | 2.62749000  | -3.24564300 | 3.93710400  |
| H | 0  | -0.15950400 | -1.12438300 | 1.07268200  |
| H | 0  | 2.30159800  | -1.44165500 | 2.29079700  |
| H | 0  | 3.89788900  | -1.81342600 | 2.47072400  |
| H | 0  | 2.59656600  | 2.95364400  | 0.52558600  |
| H | 0  | 2.25076400  | 4.44146400  | 0.61425700  |
| C | -1 | 6.23049700  | -1.68849400 | -2.13711300 |
| H | 0  | 6.79444900  | -2.17520600 | -1.33527500 |
| H | 0  | 5.85293700  | -2.46726300 | -2.80753100 |
| H | 0  | 6.94246400  | -1.08440900 | -2.71311400 |
| C | -1 | -3.30586500 | -5.21584200 | -2.49845800 |
| H | 0  | -2.59590600 | -5.94156300 | -2.91150700 |
| H | 0  | -3.96545600 | -5.75073000 | -1.80930100 |
| H | 0  | -3.90640400 | -4.83126300 | -3.32784800 |
| C | -1 | -5.90937000 | -0.36557000 | -2.33420800 |
| H | 0  | -5.32358600 | -1.23095900 | -1.97511100 |
| H | 0  | -6.96763300 | -0.60592000 | -2.17060400 |
| C | -1 | 1.94697900  | -2.97004500 | -4.18518700 |
| H | 0  | 3.04208700  | -2.98247200 | -4.17316900 |
| H | 0  | 1.62697000  | -3.23415300 | -5.19849600 |
| H | 0  | 1.62130200  | -1.94307300 | -3.98667400 |
| C | -1 | 0.76870700  | 4.68383800  | -1.36013300 |
| H | 0  | -0.14887700 | 4.89836300  | -1.92409900 |

|   |    |             |             |             |
|---|----|-------------|-------------|-------------|
| H | 0  | 1.62277500  | 5.08281600  | -1.91284100 |
| H | 0  | 0.88028700  | 3.59475200  | -1.28899500 |
| C | -1 | 2.25410100  | -0.52128500 | 5.52360500  |
| H | 0  | 1.91103900  | -0.01120100 | 6.43142800  |
| H | 0  | 2.54635200  | -1.53542000 | 5.82310700  |
| H | 0  | 3.14654800  | 0.00222300  | 5.16630000  |
| C | -1 | 1.20854700  | -5.96669500 | 3.86930700  |
| H | 0  | 1.00721800  | -7.04206500 | 3.89464000  |
| H | 0  | 2.22928900  | -5.81596400 | 4.23791700  |
| H | 0  | 0.52711700  | -5.47853000 | 4.57506300  |
| C | -1 | -4.44676000 | 3.56956100  | -0.09806500 |
| H | 0  | -4.14632900 | 4.61662300  | -0.19473100 |
| H | 0  | -3.56227700 | 2.96454100  | -0.30002100 |
| H | 0  | -5.18416800 | 3.34080200  | -0.87352000 |
| C | -1 | -1.70518800 | 2.60359300  | 3.18194600  |
| H | 0  | -0.84023300 | 2.20937400  | 3.72216600  |
| H | 0  | -2.32066200 | 3.21772800  | 3.83985600  |
| H | 0  | -2.26670300 | 1.73627400  | 2.82573900  |
| C | -1 | -0.30370600 | 1.21178200  | -4.75341700 |
| H | 0  | 0.35306900  | 2.02938200  | -4.44937700 |
| H | 0  | 0.15631000  | 0.26222000  | -4.46336000 |
| H | 0  | -1.25864000 | 1.31623000  | -4.23698500 |
| H | 0  | -0.44300800 | 1.23015500  | -5.83780300 |
| C | -1 | 4.80712700  | 4.56325200  | -2.14475200 |
| H | 0  | 5.88205000  | 4.63313200  | -1.92873000 |
| H | 0  | 4.28520300  | 4.71145400  | -1.19183200 |
| C | -1 | 3.11522500  | 5.64845000  | 3.48783400  |
| H | 0  | 4.01625300  | 6.26812900  | 3.47684800  |
| H | 0  | 3.20429300  | 4.84852700  | 2.75137000  |
| H | 0  | 2.97933100  | 5.22946600  | 4.48913600  |
| H | 0  | 2.25009900  | 6.26893300  | 3.23908100  |

H 0 3.13200400 -2.48256400 1.12243300

### 3.2 C-Lobe

TfC<sup>Phys</sup>

|   |    |             |             |             |
|---|----|-------------|-------------|-------------|
| C | 0  | 5.48867100  | -1.26319700 | 3.16143500  |
| O | 0  | 6.61021000  | -1.00972200 | 3.61393900  |
| C | 0  | 4.37432100  | 0.83672200  | 2.17005400  |
| C | 0  | 4.65685500  | 0.28596600  | 0.75726500  |
| O | -1 | 3.69755400  | -0.31725600 | 0.13472100  |
| O | 0  | 5.80636600  | 0.41666700  | 0.30593800  |
| N | 0  | 5.17974600  | -2.43873300 | 2.54317000  |
| C | 0  | -2.16568300 | -4.37014300 | -1.80319400 |
| C | 0  | -1.42970800 | -4.67079800 | -0.64468400 |
| C | 0  | -1.71952100 | -3.29985300 | -2.59396900 |
| C | 0  | -0.29566700 | -3.94435100 | -0.29669300 |
| C | 0  | -0.58950600 | -2.55362000 | -2.25285700 |
| C | 0  | 0.15436200  | -2.87252900 | -1.09867900 |
| O | -1 | 1.27058600  | -2.21295000 | -0.78303800 |
| C | 0  | 5.47754000  | 3.77566600  | -0.16391000 |
| C | 0  | 4.39252800  | 4.84448800  | 0.01088200  |
| N | 0  | 3.06309600  | 4.23622500  | 0.06478600  |
| C | 0  | 1.91687200  | 4.90736600  | 0.08870900  |
| N | 0  | 1.90429900  | 6.26165900  | 0.06729700  |
| N | 0  | 0.75886300  | 4.23131000  | 0.15644700  |
| C | 0  | 3.63927300  | -1.91577200 | -3.40482200 |
| O | 0  | 4.85523600  | -3.54749500 | -2.01972800 |
| C | 0  | -2.65840500 | 3.88819100  | -1.63242300 |
| C | 0  | -1.89960700 | 3.08108000  | -2.49787500 |
| C | 0  | -2.65756200 | 3.54533000  | -0.27205600 |

TfC<sup>Acid</sup>

|   |    |             |             |             |
|---|----|-------------|-------------|-------------|
| C | 0  | 5.48528700  | -1.08017200 | 3.18203800  |
| O | 0  | 6.60391000  | -0.77421400 | 3.60569400  |
| C | 0  | 4.30849100  | 0.96524800  | 2.15058800  |
| C | 0  | 4.61787700  | 0.39371900  | 0.75557700  |
| O | -1 | 3.67926100  | -0.25678100 | 0.13739000  |
| O | 0  | 5.76062600  | 0.54081700  | 0.30176800  |
| N | 0  | 5.20324700  | -2.28480700 | 2.60848400  |
| C | 0  | -2.09168900 | -4.47930900 | -1.70864200 |
| C | 0  | -1.36729100 | -4.71800300 | -0.52866400 |
| C | 0  | -1.64723500 | -3.43725800 | -2.54058400 |
| C | 0  | -0.24721300 | -3.95982000 | -0.19767600 |
| C | 0  | -0.53205300 | -2.66261400 | -2.21851500 |
| C | 0  | 0.20078600  | -2.91986100 | -1.04118800 |
| O | -1 | 1.30214300  | -2.23137400 | -0.74376400 |
| C | 0  | 5.37654900  | 3.87631400  | -0.25565500 |
| C | 0  | 4.26730100  | 4.92249600  | -0.10629200 |
| N | 0  | 2.95312500  | 4.28092900  | -0.04619400 |
| C | 0  | 1.79170300  | 4.92271500  | -0.01100700 |
| N | 0  | 1.74137900  | 6.27318900  | -0.05074600 |
| N | 0  | 0.65113200  | 4.21677600  | 0.09324700  |
| C | 0  | 3.66437400  | -1.88683800 | -3.32837100 |
| O | 0  | 4.89915400  | -3.51872100 | -1.96002200 |
| C | 0  | -2.76985200 | 3.75293900  | -1.74839900 |
| C | 0  | -2.00787200 | 2.92772300  | -2.59569300 |
| C | 0  | -2.73974600 | 3.46113700  | -0.37664700 |

|    |    |             |             |             |    |    |             |             |             |
|----|----|-------------|-------------|-------------|----|----|-------------|-------------|-------------|
| C  | 0  | -1.22112500 | 1.94853600  | -2.04885100 | C  | 0  | -1.30006800 | 1.82742600  | -2.11680600 |
| C  | 0  | -1.96843000 | 2.42718400  | 0.19454200  | C  | 0  | -2.02422000 | 2.37057300  | 0.11996700  |
| C  | 0  | -1.26797500 | 1.57350200  | -0.68765000 | C  | 0  | -1.32063100 | 1.49426400  | -0.74128500 |
| O  | -1 | -0.71402400 | 0.45914900  | -0.21554500 | O  | -1 | -0.74810700 | 0.40514900  | -0.24739700 |
| C  | 0  | -4.36805700 | 0.70443600  | -3.47405800 | C  | 0  | -4.39954300 | 0.44065500  | -3.42169000 |
| C  | 0  | -4.81683000 | 0.57509600  | -2.01616700 | C  | 0  | -4.67716200 | 0.34234600  | -1.91590400 |
| C  | 0  | -5.77985800 | 1.66894000  | -1.53643700 | C  | 0  | -5.54953700 | 1.48432300  | -1.40350500 |
| N  | 0  | -6.23975800 | 1.53846000  | -0.14777800 | N  | 0  | -5.68891100 | 1.44457600  | 0.09242000  |
| C  | 0  | 0.72213500  | -1.06432500 | 3.92091000  | C  | 0  | 0.71214400  | -0.97999600 | 3.93219800  |
| C  | 0  | 0.96742300  | -1.34565500 | 2.58985800  | C  | 0  | 0.91260800  | -1.30374300 | 2.60331900  |
| N  | 0  | 0.35738800  | 0.26731900  | 4.03188700  | N  | 0  | 0.40003800  | 0.36708200  | 4.01700500  |
| C  | 0  | 0.40135600  | 0.73305700  | 2.77770900  | C  | 0  | 0.43672100  | 0.80135200  | 2.75122000  |
| N  | -1 | 0.75648300  | -0.19248000 | 1.85397100  | N  | -1 | 0.72885000  | -0.16171800 | 1.84241000  |
| C  | 0  | -3.21966700 | 1.19721000  | 3.36811000  | C  | 0  | -3.14256700 | 1.18997400  | 3.44794800  |
| C  | 0  | -2.93435700 | -0.06407800 | 2.55620500  | C  | 0  | -2.78131800 | -0.04534700 | 2.62764200  |
| N  | 0  | -4.09733200 | -0.49870900 | 1.76904200  | N  | 0  | -3.91556000 | -0.47837100 | 1.78249800  |
| C  | 0  | -3.97570800 | -1.32735300 | 0.72178500  | C  | 0  | -3.74976100 | -1.43604800 | 0.83010300  |
| N  | 0  | -2.79421100 | -1.50909400 | 0.11367500  | N  | 0  | -2.59923000 | -1.57406900 | 0.18806600  |
| N  | 0  | -5.05913600 | -2.01475100 | 0.30775400  | N  | 0  | -4.81125500 | -2.21196300 | 0.55611100  |
| C  | 0  | -7.75063600 | -0.70715200 | 2.08157300  | C  | 0  | -7.85825500 | -0.45893000 | 1.85753900  |
| O  | 0  | -6.79583200 | -0.36040800 | 2.82749100  | O  | 0  | -6.84550600 | -1.08182700 | 2.27969700  |
| O  | 0  | -7.63158100 | -1.21498000 | 0.92112000  | O  | 0  | -7.85547800 | 0.38460100  | 0.89786300  |
| C  | 0  | 1.93121600  | 1.64688600  | -1.70982700 | C  | 0  | 1.85019000  | 1.62065000  | -1.77398400 |
| O  | 0  | 1.85142400  | 1.80442100  | -0.37392500 | O  | 0  | 1.79484300  | 1.80405500  | -0.43798200 |
| O  | 0  | 1.60965100  | 0.42260000  | -2.05069900 | O  | 0  | 1.56772500  | 0.37559200  | -2.07813400 |
| O  | 0  | 2.24974300  | 2.55967400  | -2.47680100 | O  | 0  | 2.12172500  | 2.52549700  | -2.56512000 |
| Fe | 0  | 1.23201900  | -0.18081600 | -0.17000000 | Fe | 0  | 1.31791900  | -0.19465000 | -0.16417900 |
| O  | 0  | 3.51134700  | -2.97281200 | 0.31154100  | O  | 0  | 3.55758100  | -2.93671800 | 0.38339300  |
| H  | 0  | 5.17406600  | 1.54149700  | 2.41351700  | H  | 0  | 5.08222700  | 1.70282100  | 2.37851200  |
| H  | 0  | 3.41387400  | 1.36193300  | 2.17393000  | H  | 0  | 3.33071400  | 1.45728400  | 2.13834700  |
| H  | 0  | 4.27966900  | -2.53435900 | 2.08161000  | H  | 0  | 4.29872600  | -2.42147200 | 2.16863800  |

|   |   |             |             |             |   |   |             |             |             |
|---|---|-------------|-------------|-------------|---|---|-------------|-------------|-------------|
| H | 0 | -1.75762600 | -5.48583400 | -0.00213000 | H | 0 | -1.69000600 | -5.51116800 | 0.14284000  |
| H | 0 | -2.26370000 | -3.04655500 | -3.49973500 | H | 0 | -2.17856800 | -3.23595600 | -3.46681100 |
| H | 0 | 0.26268700  | -4.18212200 | 0.60409100  | H | 0 | 0.30156700  | -4.15168600 | 0.71957400  |
| H | 0 | -0.25904800 | -1.72028500 | -2.86511800 | H | 0 | -0.19658400 | -1.85621400 | -2.86278000 |
| H | 0 | 6.44160300  | 4.25141900  | 0.05235100  | H | 0 | 6.32987900  | 4.38129500  | -0.06062000 |
| H | 0 | 5.34247900  | 2.99795400  | 0.59334200  | H | 0 | 5.26504800  | 3.11837600  | 0.52536600  |
| H | 0 | 4.44035800  | 5.55711400  | -0.82541900 | H | 0 | 4.30111800  | 5.61813600  | -0.95733400 |
| H | 0 | 4.56821300  | 5.40467400  | 0.93982500  | H | 0 | 4.42320100  | 5.50493600  | 0.81190800  |
| H | 0 | 2.94601800  | 3.22138100  | -0.07834100 | H | 0 | 2.86323500  | 3.26287200  | -0.17705800 |
| H | 0 | 2.76198600  | 6.76892100  | 0.21426900  | H | 0 | 2.58877400  | 6.81169900  | 0.02621300  |
| H | 0 | 1.05678600  | 6.73931200  | 0.33172600  | H | 0 | 0.88733500  | 6.73933700  | 0.21222900  |
| H | 0 | 0.84268700  | 3.21978400  | -0.03074700 | H | 0 | 0.76148500  | 3.20601900  | -0.07966700 |
| H | 0 | -0.10528300 | 4.67664100  | -0.11945300 | H | 0 | -0.21877900 | 4.63162300  | -0.21034700 |
| H | 0 | 2.73434600  | -1.99474900 | -2.79762600 | H | 0 | 2.76939900  | -1.95622400 | -2.70610000 |
| H | 0 | 3.68260600  | -0.89479000 | -3.79647100 | H | 0 | 3.70483100  | -0.86825700 | -3.72666300 |
| H | 0 | 3.56057700  | -2.61450100 | -4.24631300 | H | 0 | 3.56632800  | -2.58889900 | -4.16483400 |
| H | 0 | 4.35412900  | -3.48437500 | -1.17762600 | H | 0 | 4.40396800  | -3.45569800 | -1.11596900 |
| H | 0 | -3.21671700 | 4.15675500  | 0.43416400  | H | 0 | -3.28653100 | 4.09800200  | 0.31814100  |
| H | 0 | -1.85320100 | 3.33539300  | -3.55507000 | H | 0 | -1.98153300 | 3.14510000  | -3.66160900 |
| H | 0 | -1.95387700 | 2.19305200  | 1.25018000  | H | 0 | -1.97692000 | 2.18447300  | 1.18487100  |
| H | 0 | -0.63684600 | 1.33561200  | -2.72542100 | H | 0 | -0.71209900 | 1.20385100  | -2.78048300 |
| H | 0 | -5.24367500 | 0.66957300  | -4.13837800 | H | 0 | -5.33527700 | 0.32574300  | -3.98451700 |
| H | 0 | -3.90173200 | 1.68579500  | -3.61943400 | H | 0 | -4.01630900 | 1.44345600  | -3.64111000 |
| H | 0 | -3.92858400 | 0.59088200  | -1.37290300 | H | 0 | -3.71704800 | 0.38180200  | -1.39146600 |
| H | 0 | -5.29695000 | -0.40171100 | -1.86855300 | H | 0 | -5.14361000 | -0.62078600 | -1.67577500 |
| H | 0 | -6.66502800 | 1.69381000  | -2.18809900 | H | 0 | -6.55948500 | 1.44766000  | -1.82151000 |
| H | 0 | -5.28527200 | 2.64252600  | -1.64481900 | H | 0 | -5.09244500 | 2.43692700  | -1.67309000 |
| H | 0 | -6.73931000 | 0.65524800  | -0.03230200 | H | 0 | -6.60819500 | 0.85505600  | 0.45166300  |
| H | 0 | -5.42525200 | 1.45319700  | 0.45936800  | H | 0 | -4.84323100 | 1.06192300  | 0.53507800  |
| H | 0 | 1.30424700  | -2.25375600 | 2.10841800  | H | 0 | 1.20548400  | -2.23628200 | 2.14052200  |
| H | 0 | 0.16414400  | 1.75201100  | 2.49750900  | H | 0 | 0.23800500  | 1.82325400  | 2.45124800  |

|   |    |             |             |             |   |    |              |             |             |
|---|----|-------------|-------------|-------------|---|----|--------------|-------------|-------------|
| H | 0  | -2.25403700 | 1.52873400  | 3.76600300  | H | 0  | -2.22649200  | 1.48494400  | 3.97002400  |
| H | 0  | -3.58729900 | 1.98195400  | 2.69516700  | H | 0  | -3.40866200  | 2.01127800  | 2.77022800  |
| H | 0  | -2.61814500 | -0.87179600 | 3.23087500  | H | 0  | -2.48197900  | -0.86407000 | 3.29403800  |
| H | 0  | -2.09359500 | 0.12615100  | 1.88870200  | H | 0  | -1.92708100  | 0.17023500  | 1.98699900  |
| H | 0  | -5.04111300 | -0.45591300 | 2.19690000  | H | 0  | -4.82415300  | -0.55401900 | 2.24567400  |
| H | 0  | -6.01758000 | -1.71454100 | 0.61631500  | H | 0  | -5.68303200  | -2.03599400 | 1.06390200  |
| H | 0  | -5.00912100 | -2.40606500 | -0.62181000 | H | 0  | -4.81275800  | -2.79916800 | -0.26320700 |
| H | 0  | -2.01790400 | -0.84195600 | 0.19149300  | H | 0  | -1.85897900  | -0.83816900 | 0.17784700  |
| H | 0  | -2.73072200 | -2.15154300 | -0.66476200 | H | 0  | -2.50697100  | -2.30100300 | -0.51152000 |
| H | 0  | 3.74936000  | -2.01528800 | 0.20511800  | H | 0  | 3.78501800   | -1.98228400 | 0.25834200  |
| H | 0  | 2.58416000  | -2.92719400 | -0.02945000 | H | 0  | 2.63426300   | -2.91668700 | 0.03425800  |
| C | -1 | 4.32762600  | -0.26109700 | 3.26715500  | C | -1 | 4.29458600   | -0.11115600 | 3.26987400  |
| H | 0  | 4.39283000  | 0.21015900  | 4.25195100  | H | 0  | 4.34606200   | 0.38316000  | 4.24389800  |
| H | 0  | 3.36820600  | -0.78227600 | 3.20627200  | H | 0  | 3.35026800   | -0.66072100 | 3.22049700  |
| C | -1 | 6.15935500  | -3.45814800 | 2.17056000  | C | -1 | 6.20672800   | -3.28853000 | 2.25652000  |
| H | 0  | 7.14871100  | -3.11069000 | 2.47261800  | H | 0  | 7.19029300   | -2.89645600 | 2.52004700  |
| H | 0  | 5.94551400  | -4.41122300 | 2.66830000  | H | 0  | 6.03558500   | -4.22474400 | 2.80031000  |
| H | 0  | 6.13531600  | -3.61217000 | 1.08723900  | H | 0  | 6.16344800   | -3.49057900 | 1.18190900  |
| C | -1 | 0.86806200  | -1.98264600 | 5.10791100  | C | -1 | 0.86936100   | -1.87092500 | 5.13851900  |
| H | 0  | 1.65256500  | -1.63216100 | 5.79094000  | H | 0  | 1.70931700   | -1.54752400 | 5.76624000  |
| H | 0  | -0.05913000 | -2.05031000 | 5.69067400  | H | 0  | -0.02635900  | -1.86577200 | 5.77196800  |
| H | 0  | 1.13666300  | -2.99169300 | 4.77975600  | H | 0  | 1.06128400   | -2.90301800 | 4.82936800  |
| C | -1 | -4.20451700 | 0.99211200  | 4.51818500  | C | -1 | -4.27024900  | 0.96656200  | 4.45949800  |
| H | 0  | -4.31616500 | 1.91349500  | 5.10071100  | H | 0  | -4.44872900  | 1.87114700  | 5.04908500  |
| H | 0  | -5.19707100 | 0.69746200  | 4.16573900  | H | 0  | -5.21981900  | 0.69895000  | 3.98009800  |
| H | 0  | -3.84188000 | 0.21303300  | 5.19957500  | H | 0  | -4.01364900  | 0.15973900  | 5.15489400  |
| C | -1 | -9.19980200 | -0.48444600 | 2.58380100  | C | -1 | -9.22063400  | -0.67480700 | 2.54263600  |
| H | 0  | -9.63343800 | 0.36563900  | 2.04537000  | H | 0  | -9.40877200  | 0.16616800  | 3.21900100  |
| H | 0  | -9.81209200 | -1.36300200 | 2.36141400  | H | 0  | -10.01858700 | -0.68681600 | 1.79677600  |
| H | 0  | -9.21650300 | -0.27114300 | 3.65452000  | H | 0  | -9.22100600  | -1.59920300 | 3.12244700  |
| C | -1 | -3.50190400 | 5.03522500  | -2.14606600 | C | -1 | -3.63624700  | 4.86590100  | -2.29663400 |

|   |    |             |             |             |   |    |             |             |             |
|---|----|-------------|-------------|-------------|---|----|-------------|-------------|-------------|
| H | 0  | -4.48316500 | 4.68349300  | -2.49074500 | H | 0  | -4.57050700 | 4.47833700  | -2.72516400 |
| H | 0  | -3.68417100 | 5.78125000  | -1.36547200 | H | 0  | -3.91054600 | 5.58277700  | -1.51595900 |
| H | 0  | -3.02600800 | 5.53999500  | -2.99408900 | H | 0  | -3.12951700 | 5.41649100  | -3.09672500 |
| C | -1 | 1.34160200  | -0.21625400 | -5.44444700 | C | -1 | 1.34514200  | -0.34481500 | -5.45116000 |
| H | 0  | 0.55654000  | 0.35916500  | -5.94387700 | H | 0  | 0.47590800  | 0.08192000  | -5.96053000 |
| H | 0  | 2.25886100  | -0.17170400 | -6.03716300 | H | 0  | 2.22798000  | -0.23539000 | -6.08613500 |
| H | 0  | 1.52606300  | 0.18540300  | -4.44680000 | H | 0  | 1.50908000  | 0.15996000  | -4.49713600 |
| H | 0  | 1.02485400  | -1.25891100 | -5.35350800 | H | 0  | 1.17102000  | -1.40706400 | -5.26024900 |
| C | -1 | -3.37401100 | -0.39671800 | -3.86061600 | C | -1 | -3.37146400 | -0.60057500 | -3.88069400 |
| H | 0  | -3.01252700 | -0.28411900 | -4.88884600 | H | 0  | -3.13570800 | -0.48808100 | -4.94344500 |
| H | 0  | -2.50564200 | -0.38435300 | -3.19441100 | H | 0  | -2.44196000 | -0.50414200 | -3.31239900 |
| H | 0  | -3.84077400 | -1.38500900 | -3.77529100 | H | 0  | -3.75112300 | -1.61630700 | -3.72610700 |
| C | -1 | -3.37751200 | -5.18863300 | -2.18448200 | C | -1 | -3.26764400 | -5.35003800 | -2.09081400 |
| H | 0  | -3.09728600 | -6.19365300 | -2.52529100 | H | 0  | -2.94115900 | -6.26196600 | -2.60721500 |
| H | 0  | -4.05885000 | -5.31899500 | -1.33535100 | H | 0  | -3.83710000 | -5.66850600 | -1.21055200 |
| H | 0  | -3.94077000 | -4.71537800 | -2.99543600 | H | 0  | -3.95286500 | -4.82726500 | -2.76681400 |
| C | -1 | 4.87424900  | -2.22265300 | -2.56149200 | C | -1 | 4.91246900  | -2.19693100 | -2.50830400 |
| H | 0  | 4.96984800  | -1.47612100 | -1.76105300 | H | 0  | 5.02410000  | -1.44533300 | -1.71539700 |
| H | 0  | 5.77832500  | -2.14993700 | -3.18394400 | H | 0  | 5.80544200  | -2.13093700 | -3.14656900 |
| C | -1 | 1.71581800  | -5.06670700 | -3.29413200 | C | -1 | 1.82596600  | -5.13246400 | -3.18444800 |
| H | 0  | 1.06458600  | -5.40376200 | -2.48480800 | H | 0  | 1.18337200  | -5.40489700 | -2.34432300 |
| H | 0  | 1.91403700  | -5.89347600 | -3.98266000 | H | 0  | 2.06416100  | -6.02209200 | -3.77476600 |
| H | 0  | 1.21495000  | -4.25401400 | -3.82286300 | H | 0  | 1.29588600  | -4.40750600 | -3.80507800 |
| H | 0  | 2.65587600  | -4.69320400 | -2.88079600 | H | 0  | 2.74673900  | -4.67725700 | -2.81082700 |
| C | -1 | 5.51000500  | 3.13182400  | -1.55481300 | C | -1 | 5.41597000  | 3.19364200  | -1.62728000 |
| H | 0  | 6.20665600  | 2.29081900  | -1.55809100 | H | 0  | 6.13812400  | 2.37461000  | -1.61034700 |
| H | 0  | 4.53005400  | 2.74460700  | -1.84545500 | H | 0  | 4.44567700  | 2.76895600  | -1.89960000 |
| H | 0  | 5.81931500  | 3.86033600  | -2.31458600 | H | 0  | 5.69801600  | 3.90766700  | -2.41061000 |
|   |    |             |             |             | H | 0  | -5.80888000 | 2.38786900  | 0.46181500  |

**TfC<sub>Y517H</sub><sup>2</sup>**

|   |    |             |             |             |
|---|----|-------------|-------------|-------------|
| C | 0  | 5.45403500  | -1.00349200 | 3.18088000  |
| O | 0  | 6.57689400  | -0.67931400 | 3.57635200  |
| C | 0  | 4.30108100  | 1.01796800  | 2.10214500  |
| C | 0  | 4.60068300  | 0.41566000  | 0.72375800  |
| O | -1 | 3.65038300  | -0.25662400 | 0.11931100  |
| O | 0  | 5.72507100  | 0.53822500  | 0.23861600  |
| N | 0  | 5.17035700  | -2.22369100 | 2.64210800  |
| C | 0  | -2.11727500 | -4.52248600 | -1.63335600 |
| C | 0  | -1.39851300 | -4.72850600 | -0.44479100 |
| C | 0  | -1.67180600 | -3.50366900 | -2.49024000 |
| C | 0  | -0.28124700 | -3.96125100 | -0.13027100 |
| C | 0  | -0.56020600 | -2.71631000 | -2.18290000 |
| C | 0  | 0.16321900  | -2.94187200 | -0.99686200 |
| O | -1 | 1.26985200  | -2.24923600 | -0.71063600 |
| C | 0  | 5.38219900  | 3.87813700  | -0.38713000 |
| C | 0  | 4.27442900  | 4.92915800  | -0.24955800 |
| N | 0  | 2.96336300  | 4.29445700  | -0.09487400 |
| C | 0  | 1.80080700  | 4.93744000  | -0.09114500 |
| N | 0  | 1.75002800  | 6.28003000  | -0.22771000 |
| N | 0  | 0.66041200  | 4.24362200  | 0.08384700  |
| C | 0  | 3.60946500  | -2.00924900 | -3.27720000 |
| O | 0  | 4.93624700  | -3.59100400 | -1.93608700 |
| C | 0  | -2.78907000 | 3.72363700  | -1.85831700 |
| C | 0  | -2.01346500 | 2.88982600  | -2.68062400 |
| C | 0  | -2.79173900 | 3.45838200  | -0.48088600 |
| C | 0  | -1.32401200 | 1.79140400  | -2.16796200 |
| C | 0  | -2.09606100 | 2.36803000  | 0.04620100  |
| C | 0  | -1.39096300 | 1.49923000  | -0.79861500 |
| O | -1 | -0.77587000 | 0.40270600  | -0.28231200 |
| C | 0  | -4.41773600 | 0.35310300  | -3.41255300 |

**TfC<sub>R632H</sub><sup>Acid</sup>**

|   |    |             |             |             |
|---|----|-------------|-------------|-------------|
| C | 0  | 5.47097600  | -1.07355300 | 3.17007300  |
| O | 0  | 6.60618000  | -0.77734400 | 3.54876200  |
| C | 0  | 4.43883200  | 0.95519000  | 2.03790800  |
| C | 0  | 4.67222000  | 0.31146600  | 0.66676300  |
| O | -1 | 3.66138000  | -0.32164500 | 0.09505900  |
| O | 0  | 5.77417100  | 0.36521600  | 0.13498200  |
| N | 0  | 5.14892100  | -2.28882500 | 2.64230700  |
| C | 0  | -2.24823000 | -4.44715600 | -1.51234200 |
| C | 0  | -1.49965100 | -4.67833600 | -0.34574900 |
| C | 0  | -1.80870000 | -3.42719700 | -2.37188600 |
| C | 0  | -0.36062400 | -3.93423200 | -0.05604000 |
| C | 0  | -0.67575300 | -2.65943600 | -2.08711500 |
| C | 0  | 0.07493200  | -2.91388000 | -0.92632600 |
| O | -1 | 1.21312600  | -2.25658200 | -0.66863300 |
| C | 0  | 5.56852400  | 3.71026600  | -0.49222400 |
| C | 0  | 4.50790600  | 4.79758500  | -0.29310500 |
| N | 0  | 3.17619400  | 4.21221700  | -0.11595600 |
| C | 0  | 2.04724600  | 4.91034900  | -0.02890400 |
| N | 0  | 2.06125200  | 6.25601400  | -0.09037300 |
| N | 0  | 0.88300100  | 4.26270100  | 0.16012800  |
| C | 0  | 3.52773200  | -2.09401000 | -3.24887200 |
| O | 0  | 4.82209500  | -3.75941100 | -1.97959200 |
| C | 0  | -2.68760900 | 3.81184000  | -1.87244000 |
| C | 0  | -2.01251500 | 2.88506400  | -2.68337000 |
| C | 0  | -2.60170300 | 3.64109700  | -0.48410800 |
| C | 0  | -1.33884400 | 1.79283700  | -2.14257300 |
| C | 0  | -1.91789900 | 2.55732600  | 0.07758700  |
| C | 0  | -1.32131200 | 1.60859500  | -0.75720300 |
| O | -1 | -0.74545200 | 0.46269800  | -0.26890500 |
| C | 0  | -4.45461200 | 0.48660700  | -3.49679700 |



|    |    |             |             |             |    |    |             |             |             |
|----|----|-------------|-------------|-------------|----|----|-------------|-------------|-------------|
| C  | 0  | -4.69880100 | 0.23386100  | -1.90884000 | C  | 0  | -4.88893300 | 0.45690800  | -2.02870600 |
| C  | 0  | -5.51976900 | 1.40292300  | -1.37240700 | C  | 0  | -5.83912100 | 1.59365600  | -1.62575700 |
| N  | 0  | -5.64422700 | 1.36463900  | 0.12226000  | N  | 0  | -6.29146100 | 1.58151600  | -0.22992600 |
| C  | 0  | 0.71288600  | -0.86608700 | 3.93621200  | C  | 0  | 0.80993500  | -0.77964800 | 3.95020100  |
| C  | 0  | 0.80339000  | -1.24709000 | 2.61231800  | C  | 0  | 0.64840000  | -1.18284600 | 2.64177200  |
| N  | 0  | 0.54883400  | 0.50930100  | 3.99091600  | N  | 0  | 0.98470400  | 0.59788000  | 3.97974100  |
| C  | 0  | 0.56423600  | 0.90326900  | 2.71306800  | C  | 0  | 0.94904700  | 0.97092500  | 2.70667500  |
| N  | -1 | 0.70022200  | -0.11262100 | 1.82139800  | N  | -1 | 0.73510900  | -0.05784300 | 1.82589200  |
| C  | 0  | -3.09897000 | 1.25576800  | 3.47506100  | C  | 0  | -3.30461200 | 1.44121400  | 3.20388900  |
| C  | 0  | -2.77350000 | -0.00631100 | 2.68482800  | C  | 0  | -3.04406200 | 0.10521300  | 2.50577700  |
| N  | 0  | -3.89560500 | -0.40621200 | 1.81606800  | N  | 0  | -4.22278800 | -0.40574700 | 1.79992200  |
| C  | 0  | -3.65713400 | -1.38797100 | 0.85753500  | C  | 0  | -4.13773700 | -1.32831200 | 0.83215200  |
| N  | 0  | -2.51039300 | -1.43829700 | 0.25167200  | N  | 0  | -2.95754000 | -1.62194100 | 0.25085400  |
| N  | 0  | -4.72280700 | -2.20979500 | 0.62237000  | N  | 0  | -5.23979000 | -2.00249600 | 0.47090300  |
| C  | 0  | -7.88555200 | -0.40751000 | 1.85098800  | C  | 0  | -7.78644200 | -0.48828600 | 2.14975700  |
| O  | 0  | -6.88584200 | -1.03380400 | 2.28425000  | O  | 0  | -6.80703700 | -0.12946700 | 2.85894300  |
| O  | 0  | -7.87633100 | 0.42151500  | 0.87471900  | O  | 0  | -7.70118700 | -1.06179300 | 1.01631200  |
| C  | 0  | 1.79058200  | 1.63403600  | -1.68761100 | C  | 0  | 1.81472300  | 1.58823900  | -1.70175700 |
| O  | 0  | 1.75971700  | 1.79408000  | -0.35002300 | O  | 0  | 1.80254700  | 1.72695700  | -0.36292900 |
| O  | 0  | 1.60034500  | 0.37350600  | -2.00345700 | O  | 0  | 1.65681600  | 0.32158100  | -2.03261000 |
| O  | 0  | 1.97041500  | 2.56491600  | -2.47374900 | O  | 0  | 1.96328500  | 2.52643800  | -2.48113200 |
| Fe | 0  | 1.54194700  | -0.26742900 | -0.10305400 | Fe | 0  | 1.72202000  | -0.35923500 | -0.16669400 |
| O  | 0  | 3.54847300  | -3.02318800 | 0.39650900  | O  | 0  | 3.50025400  | -3.16030600 | 0.41300600  |
| H  | 0  | 5.09110700  | 1.74313900  | 2.31078100  | H  | 0  | 5.29493200  | 1.60768800  | 2.22297300  |
| H  | 0  | 3.33418100  | 1.52983900  | 2.07485700  | H  | 0  | 3.52590800  | 1.55640000  | 2.00074700  |
| H  | 0  | 4.24941300  | -2.39048200 | 2.25356200  | H  | 0  | 4.20681500  | -2.45135200 | 2.31060400  |
| H  | 0  | -1.72386900 | -5.50272700 | 0.24709800  | H  | 0  | -1.81674400 | -5.45594800 | 0.34550000  |
| H  | 0  | -2.20195200 | -3.32508000 | -3.42176800 | H  | 0  | -2.35807600 | -3.23256500 | -3.28812400 |
| H  | 0  | 0.26616600  | -4.13183500 | 0.79182900  | H  | 0  | 0.22038400  | -4.13469300 | 0.83941000  |
| H  | 0  | -0.22805700 | -1.92426100 | -2.84638900 | H  | 0  | -0.34007800 | -1.87637000 | -2.75953400 |
| H  | 0  | 6.33842900  | 4.39177000  | -0.23490200 | H  | 0  | 6.54802800  | 4.19064800  | -0.38887000 |

|   |   |             |             |             |   |   |             |             |             |
|---|---|-------------|-------------|-------------|---|---|-------------|-------------|-------------|
| H | 0 | 5.29273000  | 3.15216900  | 0.42693300  | H | 0 | 5.49852800  | 2.98331200  | 0.32253500  |
| H | 0 | 4.27029100  | 5.57344300  | -1.14049700 | H | 0 | 4.50256500  | 5.46546100  | -1.16623600 |
| H | 0 | 4.46779100  | 5.56370600  | 0.62559000  | H | 0 | 4.75163600  | 5.39889200  | 0.59249900  |
| H | 0 | 2.87189000  | 3.27335700  | -0.16655900 | H | 0 | 3.03927200  | 3.20318900  | -0.22289000 |
| H | 0 | 2.59697300  | 6.82439600  | -0.21347800 | H | 0 | 2.93059100  | 6.76273500  | -0.12075200 |
| H | 0 | 0.89704300  | 6.76598400  | 0.00037800  | H | 0 | 1.23542900  | 6.77667800  | 0.15871300  |
| H | 0 | 0.76487600  | 3.22373800  | -0.03157700 | H | 0 | 0.92670400  | 3.24789700  | -0.00654200 |
| H | 0 | -0.20827000 | 4.64403400  | -0.24206300 | H | 0 | 0.01896200  | 4.72149200  | -0.09263600 |
| H | 0 | 2.72641500  | -2.10920200 | -2.64197600 | H | 0 | 2.64837400  | -2.18164200 | -2.60717300 |
| H | 0 | 3.60700700  | -0.99207200 | -3.68062500 | H | 0 | 3.55300000  | -1.06719300 | -3.62534500 |
| H | 0 | 3.52691100  | -2.72010000 | -4.10709600 | H | 0 | 3.41133600  | -2.77979200 | -4.09487800 |
| H | 0 | 4.42173100  | -3.56665400 | -1.10412000 | H | 0 | 4.32467500  | -3.74952500 | -1.13969200 |
| H | 0 | -3.35685000 | 4.10433400  | 0.18875800  | H | 0 | -3.09540400 | 4.34987000  | 0.17621800  |
| H | 0 | -1.96741000 | 3.08992900  | -3.74835200 | H | 0 | -2.02300400 | 3.01367900  | -3.76243400 |
| H | 0 | -2.08164600 | 2.17864700  | 1.11101100  | H | 0 | -1.85610800 | 2.44744700  | 1.15391400  |
| H | 0 | -0.73136400 | 1.14433300  | -2.80363000 | H | 0 | -0.81044300 | 1.08283200  | -2.76730500 |
| H | 0 | -5.35296100 | 0.26010900  | -3.98047100 | H | 0 | -5.33639000 | 0.39155300  | -4.14567100 |
| H | 0 | -4.02149900 | 1.35441200  | -3.61701600 | H | 0 | -4.01056900 | 1.46388700  | -3.71867100 |
| H | 0 | -3.74122100 | 0.21206800  | -1.38091300 | H | 0 | -3.99529500 | 0.50953100  | -1.39306900 |
| H | 0 | -5.20570500 | -0.71252400 | -1.68565700 | H | 0 | -5.37334600 | -0.50352900 | -1.80797000 |
| H | 0 | -6.53536300 | 1.40537800  | -1.77982400 | H | 0 | -6.72789700 | 1.57492000  | -2.27167900 |
| H | 0 | -5.03567000 | 2.34008300  | -1.64862400 | H | 0 | -5.33807400 | 2.55154800  | -1.81761400 |
| H | 0 | -6.60849700 | 0.83791100  | 0.46715500  | H | 0 | -6.80951700 | 0.72200400  | -0.04289700 |
| H | 0 | -4.83511300 | 0.91000500  | 0.58271500  | H | 0 | -5.47772300 | 1.53110500  | 0.38115900  |
| H | 0 | 0.94237700  | -2.22294200 | 2.16807300  | H | 0 | 0.48242200  | -2.16290000 | 2.21850300  |
| H | 0 | 0.46819000  | 1.93231000  | 2.38884600  | H | 0 | 1.06666300  | 1.98994400  | 2.35822100  |
| H | 0 | -2.20032000 | 1.51137200  | 4.04737100  | H | 0 | -2.32376800 | 1.84432400  | 3.48678900  |
| H | 0 | -3.28852000 | 2.08512500  | 2.78106700  | H | 0 | -3.74276400 | 2.13872200  | 2.47934200  |
| H | 0 | -2.52291400 | -0.82104000 | 3.37885300  | H | 0 | -2.68496600 | -0.63608200 | 3.23347500  |
| H | 0 | -1.89326000 | 0.15150600  | 2.06639200  | H | 0 | -2.23635000 | 0.24746900  | 1.78886900  |
| H | 0 | -4.76897800 | -0.57418500 | 2.31439100  | H | 0 | -5.16717100 | -0.29476100 | 2.23378000  |

|   |    |              |             |             |   |    |             |             |             |
|---|----|--------------|-------------|-------------|---|----|-------------|-------------|-------------|
| H | 0  | -5.61744400  | -1.98152600 | 1.05646300  | H | 0  | -6.19692700 | -1.63939800 | 0.74738400  |
| H | 0  | -4.72539900  | -2.75347300 | -0.22643900 | H | 0  | -5.19632300 | -2.50095400 | -0.40618000 |
| H | 0  | -2.45340400  | -2.19067100 | -0.42806800 | H | 0  | -2.18380800 | -0.96821200 | 0.25590600  |
| H | 0  | 3.83025100   | -2.09350900 | 0.26452000  | H | 0  | -2.92885000 | -2.30049000 | -0.49863500 |
| H | 0  | 2.62947800   | -2.97319200 | 0.03751500  | H | 0  | 3.84206700  | -2.25743700 | 0.27184600  |
| C | -1 | 4.26616200   | -0.03133700 | 3.24697900  | H | 0  | 2.58372200  | -3.06980500 | 0.06466200  |
| H | 0  | 4.31544100   | 0.48977200  | 4.20629800  | C | -1 | 4.32050900  | -0.05600800 | 3.21078000  |
| H | 0  | 3.31617000   | -0.57258600 | 3.20606600  | H | 0  | 4.37511600  | 0.48916100  | 4.15525900  |
| C | -1 | 6.17283300   | -3.23703000 | 2.31583400  | H | 0  | 3.34896800  | -0.55604400 | 3.16459400  |
| H | 0  | 7.15708300   | -2.82928900 | 2.55060200  | C | -1 | 6.11959700  | -3.33439900 | 2.32016900  |
| H | 0  | 6.01352200   | -4.15090000 | 2.89906700  | H | 0  | 7.12081500  | -2.92055400 | 2.44849500  |
| H | 0  | 6.11681900   | -3.48201600 | 1.25102500  | H | 0  | 6.00453100  | -4.20145100 | 2.98038500  |
| C | -1 | 0.83807900   | -1.73651500 | 5.16044000  | H | 0  | 5.97932400  | -3.65523500 | 1.28464800  |
| H | 0  | 1.73033600   | -1.47633100 | 5.74360800  | C | -1 | 0.86631500  | -1.62092300 | 5.19536300  |
| H | 0  | -0.02573800  | -1.63124600 | 5.82845000  | H | 0  | 1.84863200  | -1.54227500 | 5.67644000  |
| H | 0  | 0.91923800   | -2.78938900 | 4.87368700  | H | 0  | 0.11907300  | -1.30329200 | 5.93196600  |
| C | -1 | -4.29675100  | 1.09126100  | 4.40861500  | H | 0  | 0.68777800  | -2.67407800 | 4.95930300  |
| H | 0  | -4.46939000  | 1.99840000  | 4.99725200  | C | -1 | -4.19085700 | 1.34502000  | 4.44660300  |
| H | 0  | -5.22318500  | 0.87765800  | 3.86257000  | H | 0  | -4.28930100 | 2.32456000  | 4.92585200  |
| H | 0  | -4.13323000  | 0.26619200  | 5.11156400  | H | 0  | -5.19525100 | 0.98781200  | 4.20086400  |
| C | -1 | -9.25000100  | -0.59055100 | 2.53477600  | H | 0  | -3.75276500 | 0.65747600  | 5.17935200  |
| H | 0  | -9.45075600  | 0.28590100  | 3.16081400  | C | -1 | -9.21400700 | -0.22236200 | 2.66130700  |
| H | 0  | -10.04250800 | -0.64764300 | 1.78443600  | H | 0  | -9.72835400 | 0.44161200  | 1.95907100  |
| H | 0  | -9.25402800  | -1.48228800 | 3.16383100  | H | 0  | -9.77291800 | -1.16286900 | 2.68891100  |
| C | -1 | -3.65656400  | 4.81403000  | -2.44581000 | H | 0  | -9.20329800 | 0.23306600  | 3.65342000  |
| H | 0  | -4.59898200  | 4.40289700  | -2.83045000 | C | -1 | -3.52106100 | 4.91683500  | -2.48505100 |
| H | 0  | -3.91294200  | 5.57204400  | -1.69910900 | H | 0  | -4.49348400 | 4.53222300  | -2.81576100 |
| H | 0  | -3.16303300  | 5.31572300  | -3.28449300 | H | 0  | -3.71469400 | 5.71995600  | -1.76784800 |
| C | -1 | 1.31575000   | -0.48472800 | -5.46507000 | H | 0  | -3.02939500 | 5.35090800  | -3.36184300 |
| H | 0  | 0.41837900   | -0.11770000 | -5.97159600 | C | -1 | 1.25499500  | -0.58508700 | -5.45739200 |
| H | 0  | 2.19504800   | -0.25892300 | -6.07350500 | H | 0  | 0.39873600  | -0.16372000 | -5.99161100 |

|   |    |             |             |             |   |    |             |             |             |
|---|----|-------------|-------------|-------------|---|----|-------------|-------------|-------------|
| H | 0  | 1.41554300  | -0.01087600 | -4.48622100 | H | 0  | 2.15217900  | -0.48865500 | -6.07374300 |
| H | 0  | 1.24148300  | -1.56643100 | -5.32802400 | H | 0  | 1.40243700  | -0.06100300 | -4.51067800 |
| C | -1 | -3.40121700 | -0.69188500 | -3.88837600 | H | 0  | 1.07292900  | -1.64305400 | -5.25225300 |
| H | 0  | -3.16654300 | -0.56842400 | -4.95042000 | C | -1 | -3.44686000 | -0.62065100 | -3.82411600 |
| H | 0  | -2.46947400 | -0.61475900 | -3.32045400 | H | 0  | -3.09216700 | -0.56176800 | -4.85885300 |
| H | 0  | -3.78939000 | -1.70593800 | -3.74476000 | H | 0  | -2.57611000 | -0.56357700 | -3.16411200 |
| C | -1 | -3.30531300 | -5.39380000 | -1.97670600 | H | 0  | -3.90123700 | -1.60777100 | -3.68177700 |
| H | 0  | -2.99089200 | -6.37449700 | -2.35625700 | C | -1 | -3.46867000 | -5.28646200 | -1.82350800 |
| H | 0  | -3.93444100 | -5.57811500 | -1.09846500 | H | 0  | -3.18970400 | -6.30743600 | -2.11130200 |
| H | 0  | -3.93045000 | -4.93308700 | -2.74868600 | H | 0  | -4.12985700 | -5.36815800 | -0.95334200 |
| C | -1 | 4.88011800  | -2.26642800 | -2.47551500 | H | 0  | -4.04738100 | -4.85982400 | -2.64849000 |
| H | 0  | 4.97858500  | -1.51197900 | -1.68339400 | C | -1 | 4.80011100  | -2.41626000 | -2.47420000 |
| H | 0  | 5.75893400  | -2.16028000 | -3.12705100 | H | 0  | 4.93672900  | -1.69165000 | -1.65929100 |
| C | -1 | 1.78858300  | -5.21316000 | -3.07569000 | H | 0  | 5.67233100  | -2.31620300 | -3.13433000 |
| H | 0  | 1.13841100  | -5.43189200 | -2.22602900 | C | -1 | 1.61511800  | -5.27957300 | -2.98288100 |
| H | 0  | 1.96647600  | -6.12474000 | -3.65358400 | H | 0  | 1.03605600  | -5.53255600 | -2.09197100 |
| H | 0  | 1.29827800  | -4.46629900 | -3.70275300 | H | 0  | 1.73726300  | -6.16743200 | -3.60951700 |
| H | 0  | 2.73916800  | -4.80962100 | -2.71894300 | H | 0  | 1.07939100  | -4.50644500 | -3.53677500 |
| C | -1 | 5.39283800  | 3.14420400  | -1.73376500 | H | 0  | 2.59537500  | -4.89583600 | -2.69047500 |
| H | 0  | 6.11454100  | 2.32536300  | -1.70531800 | C | -1 | 5.48248000  | 2.98965600  | -1.84251100 |
| H | 0  | 4.41402800  | 2.71421900  | -1.96725800 | H | 0  | 6.18899200  | 2.15741300  | -1.87061200 |
| H | 0  | 5.65679200  | 3.82913600  | -2.54818600 | H | 0  | 4.48341800  | 2.58019100  | -2.02339300 |
| H | 0  | -5.69421200 | 2.31152500  | 0.49723100  | H | 0  | 5.70930800  | 3.67742700  | -2.66529300 |
| H | 0  | -1.46364200 | -0.32685600 | 0.02478000  | H | 0  | -0.41975000 | 0.51991500  | 0.66889100  |