Name Surname :____Teacher________________________________ Group Nº __Teacher__2025

**Enzyme Proteins A.**Task **liver** CATALASE studies for student practical introduction helping material:

ChemScape MDLi **RasMol** MAGE FireFox application. **B.**Lunch Kenyon University: http://aris.gusc.lv/ChemFiles/catalaseKenyon/cat1.htm professor Elizabeth M. Boon '97, Aaron Downs '00, David Marcey and Aris Kaksis 2025 Riga Stradin's University prepared molecular tutorial

**1.** Call the cell organelles where first enzyme CATALASE found and classification number!
**EC1.11.1.6**..............................organelles peroxisomes.............................

**2** High rate protolysis activate $G_{H2O}+G_{HOOH}=0+365=365$ $^{kJ}/_{mol}$ to $G_{H3O+}+G_{HOO-}=22.44+418.32=440.76$ $^{kJ}/_{mol}$;

**1)** Protolysis **HOOH**+$H_2O$⇔$H_3O^+$+$HOO^-$ $pK_a=11{,}75$ make possible collisions of anions **$HOO^-$><$^-$OOH**.

**2)** High activation energy $E_a=79000$ $^{J}/_{mol}$ colliding **$HOO^-$><$^-$OOH** with slow velocity $\vec{k}=1.416*10^{-16}$ $M^{-2}s^{-1}$ constant disproportionate **$^-$OOH** oxidize atoms to $O_{2aqua}$ and second atoms **$^-$OOH** reduce about 2 $OH^-$ ions,

**3)** which neutralizing to water: $2OH^-+2H_3O^+\Rightarrow 2H_2O+2H_2O$. In summary produce $O_{2aqua}+2H_2O+2H_2O+Q$:

$2H_2O_2+2H_2O \rightarrow H_3O^+ + HOO^- >< {}^-OOH + H_3O^+ \rightarrow O_{2aqua}+2H_2O+2H_2O+Q$ the Life resources...................... .

**2.a** Collision negative to positive $HOO^->Fe^{3+}$ have $E_a=29$ $^{J}/_{mol}$ indispensible law activation energy with protonation the **His74** and Asn 147 velocity constant increases over absent **CATALASE** 30 million times as geometric factor **A** improve to **A**=>0.131: $H_2O_2+H_2O_2+Fe^{3+} \rightarrow$ His74-$H^+$+$HOO^->Fe^{3+}<{}^-OOH$+ Asn147-$H^+$$\rightarrow O_{2aqua}+H_2O+H_2O+Q_{exothermic}+Fe^{3+}$.

Protolysis activate transition state complex **oxygen**+ **water**+ **heat**+ CATALASE,

Negative anions collisions with positive iron $Fe^{3+}$ ion produce life resources 30 million times faster.

Write disproportionation reaction first and second peroxide molecule:

1. **H-O-O-H**$_{protolysis}$+**Fe(III)**+**His74**=>**Fe(IV)-O**+(**$HO^-$**$_{Red}$+**$H^+$**$_{protonation}$-**His74**=>**$H_2O$**).......................
2. **H-O-O-H**$_{protolysis}$+**Fe(IV)-O**$_{Ox}$+ Asn147=>**Fe(III)**+**O=O**$_{Ox}$+(**$HO^-$**$_{Red}$+**$H^+$**$_{protonation}$- Asn147=>**$H_2O$**)..................

**3.** Two non enzymatic and Biochemical peroxide sources in oxygen dissolute water !

1) Heavy metal compounds iron $Fe^{3+}$....., cooper $Cu^{2+}$…., manganesium $Mn^{4+}$...., lead $Pb^{4+}$....

2) Ionization radiation: ultraviolet UV radiation..............., roentgen x-ray radiation................, gamma **γ** radiation.............,beta ($\beta^-$un$\beta^+$)radiation..................,alpha particles $\alpha^{2+}$ radiation.......

3) **Peroxisomal** ethylene **-$CH_2$-$CH_2$-** dehydrogenation to cis double bond **H>C=C<H**..............

**4.** What **N-terminus** Asn3... and C-terminus Asn500.... amino acids have **8CAT.pdb**?
What number of amino acid has **CATALASE** polypeptide chain? 527......
What is number of amino acids on chain of **8CAT.pdb** 500-3=497; 497+1= 498.........?

**4a 1-4.** What **8CAT.pdb** isoelectric point IEP=pH=$pK_{a\text{-}vid}$ , total charge at pH=7,36 ?
To determine water solution pH with **CATALASE** concentration $C=10^{-7{,}021667}$ M ($^{mol}/_{Litre}$)!

Liver Catalase (EC 1.11.1.6), present in the peroxisomes

```
   SQ SEQUENCE 527 >8CAT:A|PDBID|CHAIN|SEQUENCE 67527,6 g/mol
MADNRDPASDQMKHWKEQRAAQKPDVLTTGGGNPVGDKLNSLTVGPRGPLLVQDVVFTDEMAHFDRERIPERVVHAKGAG
AFGYFEVTHDITRYSKAKVFEHIGKRTPIAVRFSTVAGESGSADTVRDPRGFAVKFYTEDGNWDLVGNNTPIFFIRDALL
FPSFIHSQKRNPQTHLKDPDMVWDFWSLRPESLHQVSFLFSDRGIPDGHRHMNGYGSHTFKLVNANGEAVYCKFHYKTDQ
GIKNLSVEDAARLAHEDPDYGLRDLFNAIATGNYPSWTLYIQVMTFSEAEIFPFNPFDLTKVWPHGDYPLIPVGKLVLNR
NPVNYFAEVEQLAFDPSNMPPGIEPSPDKMLQGRLFAYPDTHRHRLGPNYLQIPVNCPYRARVANYQRDGPMCMMDNQGG
APNYYPNSFSAPEHQPSALEHRTHFSGDVQRFNSANDDNVTQVRTFYLKVLNEEQRKRLCENIAGHLKDAQLFIQKKAVK
NFSDVHPEYGSRIQALLDKYNEEKPKNAVHTYVQHGSHLSAREKANL
        10         20         30         40         50         60         70         80
MADNRDPASD QMKHWKEQRA AQKPDVLTTG GGNPVGDKLN SLTVGPRGPL LVQDVVFTDE MAHFDRERIP ERVVHAKGAG
        90        100        110        120        130        140        150        160
AFGYFEVTHD ITRYSKAKVF EHIGKRTPIA VRFSTVAGES GSADTVRDPR GFAVKFYTED GNWDLVGNNT PIFFIRDALL
       170        180        190        200        210        220        230        240
FPSFIHSQKR NPQTHLKDPD MVWDFWSLRP ESLHQVSFLF SDRGIPDGHR HMNGYGSHTF KLVNANGEAV YCKFHYKTDQ
       250        260        270        280        290        300        310        320
GIKNLSVEDA ARLAHEDPDY GLRDLFNAIA TGNYPSWTLY IQVMTFSEAE IFPFNPFDLT KVWPHGDYPL IPVGKLVLNR
       330        340        350        360        370        380        390        400
NPVNYFAEVE QLAFDPSNMP PGIEPSPDKM LQGRLFAYPD THRHRLGPNY LQIPVNCPYR ARVANYQRDG PMCMMDNQGG
       410        420        430        440        450        460        470        480
APNYYPNSFS APEHQPSALE HRTHFSGDVQ RFNSANDDNV TQVRTFYLKV LNEEQRKRLC ENIAGHLKDA QLFIQKKAVK
       490        500        510        520       527
NFSDVHPEYG SRIQALLDKY NEEKPKNAVH TYVQHGSHLS AREKANL     CATA_BOVIN
```

$pK_{mean}=pK_{sum}/$ NpK =1339,51........../174...........=............... pKa count 172....+2....=.174..........=NpK

Val73,Val74,Ala76,Val116,Ala117,Pro129,Gly131,Val146,Gly147,Phe153,Phe154,Ile155,
Ala158,Leu159,Leu160,Phe161,Pro162,Phe164,Ile165,Phe198,Leu199,Phe200,
Leu299,Ala333,Phe334,Pro336,Met350,Leu351,Gly353,Phe356,Ala357,Pro359,Ala435
Val72,Val73,Ala75,Val115,Ala116,Pro128,Gly130,Val145,Gly146,Phe152,Phe153,Ile154,shift -1
Ala157,Leu158,Leu159,Phe160,Pro161,Phe163,Ile164,Phe197,Leu198,Phe199,
Leu298,Ala332,Phe333,Pro335,Met349,Leu350,Gly352,Phe355,Ala356,Pro358,Ala434

In account are present four Cysteine residues $pK_{RR}$ =8.18; Sum of 174 pKa in table sum ..................

| AA | $pKa_{COO^-}$ | $pKa_{NH3^+}$ | $pK_{RR}$ | Nr | | AA | $pKa_{COO^-}$ | $pKa_{NH3^+}$ | $pK_{RR}$ | Nr | | AA | $pKa_{COO^-}$ | $pKa_{NH3^+}$ | $pK_{RR}$ | Nr | | AA | $pKa_{COO^-}$ | $pKa_{NH3^+}$ | $pK_{RR}$ | Nr | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A | -- | 9,69 | | 1 | 1 | R | | | 12,48 | 129 | 45 | D | | | 3,65 | 256 | 89 | E | | | 4,25 | 419 | 133 |
| D | -- | | 3,65 | 2 | 2 | K | | | 10,53 | 134 | 46 | D | | | 3,65 | 258 | 90 | H | | | 6 | 420 | 134 |
| R | -- | | 12,48 | 4 | 3 | Y | | | 10,07 | 136 | 47 | Y | | | 10,07 | 259 | 91 | R | | | 12,48 | 421 | 135 |
| D | -- | | 3,65 | 5 | 4 | E | | | 4,25 | 138 | 48 | R | | | 12,48 | 262 | 92 | H | | | 6 | 423 | 136 |
| D | -- | | 3,65 | 9 | 5 | D | | | 3,65 | 139 | 49 | D | | | 3,65 | 263 | 93 | D | | | 3,65 | 427 | 137 |
| K | -- | | 10,53 | 12 | 6 | D | | | 3,65 | 143 | 50 | Y | | | 10,07 | 273 | 94 | R | | | 12,48 | 430 | 138 |
| H | -- | | 6 | 13 | 7 | R | | | 12,48 | 155 | 51 | Y | | | 10,07 | 279 | 95 | D | | | 3,65 | 436 | 139 |
| K | -- | | 10,53 | 15 | 8 | D | | | 3,65 | 156 | 52 | E | | | 4,25 | 287 | 96 | D | | | 3,65 | 437 | 140 |
| E | -- | | 4,25 | 16 | 9 | H | | | 6 | 165 | 53 | E | | | 4,25 | 289 | 97 | R | | | 12,48 | 443 | 141 |
| R | -- | | 12,48 | 18 | 10 | K | | | 10,53 | 168 | 54 | D | | | 3,65 | 297 | 98 | Y | | | 10,07 | 446 | 142 |
| K | -- | | 10,53 | 22 | 11 | R | | | 12,48 | 169 | 55 | K | | | 10,53 | 300 | 99 | K | | | 10,53 | 448 | 143 |
| D | -- | | 3,65 | 24 | 12 | H | | | 6 | 174 | 56 | H | | | 6 | 304 | 100 | E | | | 4,25 | 452 | 144 |
| D | -- | | 3,65 | 36 | 13 | K | | | 10,53 | 176 | 57 | D | | | 3,65 | 306 | 101 | E | | | 4,25 | 453 | 145 |
| K | -- | | 10,53 | 37 | 14 | D | | | 3,65 | 177 | 58 | Y | | | 10,07 | 307 | 102 | R | | | 12,48 | 455 | 146 |
| R | -- | | 12,48 | 46 | 15 | D | | | 3,65 | 179 | 59 | K | | | 10,53 | 314 | 103 | K | | | 10,53 | 456 | 147 |
| D | -- | | 3,65 | 53 | 16 | D | | | 3,65 | 183 | 60 | R | | | 12,48 | 319 | 104 | R | | | 12,48 | 457 | 148 |
| D | -- | | 3,65 | 58 | 17 | R | | | 12,48 | 188 | 61 | Y | | | 10,07 | 324 | 105 | C | | | 8,18 | 459 | 149 |
| E | -- | | 4,25 | 59 | 18 | E | | | 4,25 | 190 | 62 | E | | | 4,25 | 327 | 106 | E | | | 4,25 | 460 | 150 |
| H | -- | | 6 | 62 | 19 | H | | | 6 | 193 | 63 | E | | | 4,25 | 329 | 107 | H | | | 6 | 465 | 151 |
| D | -- | | 3,65 | 64 | 20 | D | | | 3,65 | 201 | 64 | D | | | 3,65 | 334 | 108 | K | | | 10,53 | 467 | 152 |
| R | -- | | 12,48 | 65 | 21 | R | | | 12,48 | 202 | 65 | E | | | 4,25 | 343 | 109 | D | | | 3,65 | 468 | 153 |
| E | -- | | 4,25 | 66 | 22 | D | | | 3,65 | 206 | 66 | D | | | 3,65 | 347 | 110 | K | | | 10,53 | 475 | 154 |
| R | -- | | 12,48 | 67 | 23 | H | | | 6 | 208 | 67 | K | | | 10,53 | 348 | 111 | K | | | 10,53 | 476 | 155 |
| E | -- | | 4,25 | 70 | 24 | R | | | 12,48 | 209 | 68 | R | | | 12,48 | 353 | 112 | K | | | 10,53 | 479 | 156 |
| R | -- | | 12,48 | 71 | 25 | H | | | 6 | 210 | 69 | Y | | | 10,07 | 357 | 113 | D | | | 3,65 | 484 | 157 |
| H | -- | | 6 | 74 | 26 | D | | | 3,65 | 212 | 70 | D | | | 3,65 | 359 | 114 | H | | | 6 | 486 | 158 |
| K | -- | | 10,53 | 76 | 27 | Y | | | 10,07 | 214 | 71 | H | | | 6 | 361 | 115 | E | | | 4,25 | 488 | 159 |
| Y | -- | | 10,07 | 83 | 28 | H | | | 6 | 217 | 72 | R | | | 12,48 | 362 | 116 | Y | | | 10,07 | 489 | 160 |
| E | -- | | 4,25 | 85 | 29 | K | | | 10,53 | 220 | 73 | H | | | 6 | 363 | 117 | R | | | 12,48 | 492 | 161 |
| H | -- | | 6 | 88 | 30 | D | | | 3,65 | 225 | 74 | R | | | 12,48 | 364 | 118 | D | | | 3,65 | 498 | 162 |
| D | -- | | 3,65 | 89 | 31 | E | | | 4,25 | 227 | 75 | Y | | | 10,07 | 369 | 119 | K | | | 10,53 | 499 | 163 |
| R | -- | | 12,48 | 92 | 32 | Y | | | 10,07 | 230 | 76 | C | | | 8,18 | 376 | 120 | Y | | | 10,07 | 500 | 164 |
| Y | -- | | 10,07 | 93 | 33 | C | | | 8,18 | 231 | 77 | Y | | | 10,07 | 378 | 121 | E | | | 4,25 | 502 | 165 |
| K | -- | | 10,53 | 95 | 34 | K | | | 10,53 | 232 | 78 | R | | | 12,48 | 379 | 122 | E | | | 4,25 | 503 | 166 |
| K | -- | | 10,53 | 97 | 35 | H | | | 6 | 234 | 79 | R | | | 12,48 | 381 | 123 | K | | | 10,53 | 504 | 167 |
| E | -- | | 4,25 | 100 | 36 | Y | | | 10,07 | 235 | 80 | Y | | | 10,07 | 385 | 124 | K | | | 10,53 | 506 | 168 |
| H | -- | | 6 | 101 | 37 | K | | | 10,53 | 236 | 81 | R | | | 12,48 | 387 | 125 | H | | | 6 | 510 | 169 |
| K | -- | | 10,53 | 104 | 38 | D | | | 3,65 | 238 | 82 | D | | | 3,65 | 388 | 126 | Y | | | 10,07 | 512 | 170 |
| R | -- | | 12,48 | 105 | 39 | K | | | 10,53 | 242 | 83 | C | | | 8,18 | 392 | 127 | H | | | 6 | 515 | 171 |
| R | -- | | 12,48 | 111 | 40 | E | | | 4,25 | 247 | 84 | D | | | 3,65 | 395 | 128 | H | | | 6 | 518 | 172 |
| E | -- | | 4,25 | 118 | 41 | D | | | 3,65 | 248 | 85 | Y | | | 10,07 | 403 | 129 | R | | | 12,48 | 522 | 173 |
| D | -- | | 3,65 | 123 | 42 | R | | | 12,48 | 251 | 86 | Y | | | 10,07 | 404 | 130 | E | | | 4,25 | 523 | 174 |
| R | -- | | 12,48 | 126 | 43 | H | | | 6 | 254 | 87 | E | | | 4,25 | 412 | 131 | K | | | 10,53 | 524 | 175 |
| D | -- | | 3,65 | 127 | 44 | E | | | 4,25 | 255 | 88 | H | | | 6 | 413 | 132 | L | 2,36 | | | 527 | 176 |

Tasks for catalase molecule 8CAT.pdb

Protolytic constant $pK_a$ isoelectric point IEP=$pK_a$ calculate of side chains $\Sigma pK_{aRside\ group}$ ; Nterminal $pK_{aNterminal}NH_3^+$ and $pK_{aCterminal}COO^-$ constants sum divide with number of acid groups $NpK_a$:

$$IEP=pK_a=(\Sigma pKa_{Rside\ group}+pKa_{Nterminal}+pKa_{Cterminal})/NpKa$$

Acid groups number in sum NpKa=172.......+2.........= 174.....

527 amino acids of them for $pK_a$ side groups number 172+2.

N-terminal Methionine M $pK_{aNterminal}$=9.21 and

C-terminal Lysine K $pKa_{Cterminal}$=2.34

Sum are calculate as

$\Sigma pKa=\Sigma pKa_{Rside\ group}+pK_{aNterminal}+pKa_{Cterminala}$=1339,51..........

**1.** Average constant $pK_{mean}=pK_a$=IEP **ISOELEKTRIC POINT**

NpKa=172.......+2........=174........ ;

IEP=ΣpKa/ NpKa =1339,51/ 174 =**7,698333**.............

At pH value on isoelectric point pH**=IEP total charge** is zero „**0**"

zero charge „**0**" **IEP**=pH

**COOH** & **-$NH_3^+$** positive **$COO^-$** & **$NH_3^+$** negative **-$COO^-$** & **-$NH_2$**

Underline existing!

**2.** 8CAT molecule charge sign (**+**). zero „**0**" or (**-**) at pH=7.36

Underline existing:

**COOH**,**$NH_3^+$** positive + pH=7.36<IEP=**7,7** negative-**$COO^-$**,**$NH_2$**.

**3.** 8CAT molecule charge **+**. zero „**0**" or **-** at **electrophoresis** pH **8.8**

Underline existing:

**COOH**,**$NH_3^+$** positive +IEP=**7,7**<pH = **8,8** negative **-** **$COO^-$**,**$NH_2$**

**4.** Calculate solution pH $C=10^{-7,021667}$ M 8CAT by *Ostwald dilution law*

concentration C in logarithm:

$$pH=\frac{pK_a-\log C}{2}=\frac{7,698333-\log 10^{-7,021667}}{2}=\frac{7,698333+7,021667}{2}=\mathbf{14,7201}/2=7,36......$$

Attractor 7,36 concentration of 8CAT is $10^{-7,021667}$..........M.

**4b.** What **1QQW.pdb** isoelectric point IEP=pH=$pK_{a\text{-}vid}$ at physiologic pH=7,36 ? To determine water solution pH with **CATALASE** concentration $C=10^{-7,021667}$ M ($^{mol}/_{Litre}$)!

# Catalase (EC 1.11.1.6), present in Human erytrocites

```
    SQ SEQUENCE 527 >1QQW:A|PDBID|CHAIN|SEQUENCE 67384,637 g/mol
MADSRDPASDQMQHWKEQRAAQKADVLTTGAGNPVGDKLNVITVGPRGPLLVQDVVFTDEMAHFDRERIPERVVHAKGAG
AFGYFEVTHDITKYSKAKVFEHIGKKTPIAVRFSTVAGESGSADTVRDPRGFAVKFYTEDGNWDLVGNNTPIFFIRDPIL
FPSFIHSQKRNPQTHLKDPDMVWDFWSLRPESLHQVSFLFSDRGIPDGHRHMNGYGSHTFKLVNANGEAVYCKFHYKTDQ
GIKNLSVEDAARLSQEDPDYGIRDLFNAIATGKYPSWTFYIQVMTFNQAETFPFNPFDLTKVWPHKDYPLIPVGKLVLNR
NPVNYFAEVEQIAFDPSNMPPGIEASPDKMLQGRLFAYPDTHRHRLGPNYLHIPVNCPYRARVANYQRDGPMCMQDNQGG
APNYYPNSFGAPEQQPSALEHSIQYSGEVRRFNTANDDNVTQVRAFYVNVLNEEQRKRLCENIAGHLKDAQIFIQKKAVK
NFTEVHPDYGSHIQALLDKYNAEKPKNAIHTFVQSGSHLAAREKANL
```

| AA | $pKa_{COO-}$ | $pKa_{NH3+}$ | $pK_{RR}$ | | Nr |
|---|---|---|---|---|---|
| M | -- | 9,21 | | 1 | 1 |
| D | -- | | 3,65 | 3 | 2 |
| R | -- | | 12,48 | 5 | 3 |
| D | -- | | 3,65 | 6 | 4 |
| D | -- | | 3,65 | 10 | 5 |
| K | -- | | 10,53 | 13 | 6 |
| H | -- | | 6 | 14 | 7 |
| K | -- | | 10,53 | 16 | 8 |
| E | -- | | 4,25 | 17 | 9 |
| R | -- | | 12,48 | 19 | 10 |
| K | -- | | 10,53 | 23 | 11 |
| D | -- | | 3,65 | 25 | 12 |
| D | -- | | 3,65 | 37 | 13 |
| K | -- | | 10,53 | 38 | 14 |
| R | -- | | 12,48 | 47 | 15 |
| D | -- | | 3,65 | 54 | 16 |
| D | -- | | 3,65 | 59 | 17 |
| E | -- | | 4,25 | 60 | 18 |
| H | -- | | 6 | 63 | 19 |
| D | -- | | 3,65 | 65 | 20 |
| R | -- | | 12,48 | 66 | 21 |
| E | -- | | 4,25 | 67 | 22 |
| R | -- | | 12,48 | 68 | 23 |
| E | -- | | 4,25 | 71 | 24 |
| R | -- | | 12,48 | 72 | 25 |
| H | -- | | 6 | 75 | 26 |
| K | -- | | 10,53 | 77 | 27 |
| Y | -- | | 10,07 | 84 | 28 |
| E | -- | | 4,25 | 86 | 29 |
| H | -- | | 6 | 89 | 30 |
| D | -- | | 3,65 | 90 | 31 |
| R | -- | | 12,48 | 93 | 32 |
| Y | -- | | 10,07 | 94 | 33 |
| K | -- | | 10,53 | 96 | 34 |
| K | -- | | 10,53 | 98 | 35 |
| E | -- | | 4,25 | 101 | 36 |
| H | -- | | 6 | 102 | 37 |
| K | -- | | 10,53 | 105 | 38 |
| R | -- | | 12,48 | 106 | 39 |
| R | -- | | 12,48 | 112 | 40 |
| E | -- | | 4,25 | 119 | 41 |
| D | -- | | 3,65 | 124 | 42 |
| R | -- | | 12,48 | 127 | 43 |
| D | -- | | 3,65 | 128 | 44 |
| K | -- | | 10,53 | 135 | 45 |
| Y | -- | | 10,07 | 137 | 46 |
| E | -- | | 4,25 | 139 | 47 |
| D | -- | | 3,65 | 140 | 48 |
| D | -- | | 3,65 | 144 | 49 |
| R | -- | | 12,48 | 156 | 50 |
| D | -- | | 3,65 | 157 | 51 |
| H | -- | | 6 | 166 | 52 |
| K | -- | | 10,53 | 169 | 53 |
| R | -- | | 12,48 | 170 | 54 |
| H | -- | | 6 | 175 | 55 |
| K | -- | | 10,53 | 177 | 56 |
| D | -- | | 3,65 | 178 | 57 |
| D | -- | | 3,65 | 180 | 58 |
| D | -- | | 3,65 | 184 | 59 |
| R | -- | | 12,48 | 189 | 60 |
| E | -- | | 4,25 | 191 | 61 |
| H | -- | | 6 | 194 | 62 |
| D | -- | | 3,65 | 202 | 63 |
| R | -- | | 12,48 | 203 | 64 |
| D | -- | | 3,65 | 207 | 65 |
| H | -- | | 6 | 209 | 66 |
| R | -- | | 12,48 | 210 | 67 |
| H | -- | | 6 | 211 | 68 |
| Y | -- | | 10,07 | 215 | 69 |
| H | -- | | 6 | 218 | 70 |
| K | -- | | 10,53 | 221 | 71 |
| E | -- | | 4,25 | 228 | 72 |
| Y | -- | | 10,07 | 231 | 73 |
| C | -- | | 8,18 | 232 | 74 |
| K | -- | | 10,53 | 233 | 75 |
| H | -- | | 6 | 235 | 76 |
| Y | -- | | 10,07 | 236 | 77 |
| K | -- | | 10,53 | 237 | 78 |
| D | -- | | 3,65 | 239 | 79 |
| K | -- | | 10,53 | 243 | 80 |
| E | -- | | 4,25 | 248 | 81 |
| D | -- | | 3,65 | 249 | 82 |
| R | -- | | 12,48 | 252 | 83 |
| E | -- | | 4,25 | 256 | 84 |
| D | -- | | 3,65 | 257 | 85 |
| D | -- | | 3,65 | 259 | 86 |
| Y | -- | | 10,07 | 260 | 87 |
| R | -- | | 12,48 | 263 | 88 |
| D | -- | | 3,65 | 264 | 89 |
| K | -- | | 10,53 | 273 | 90 |
| Y | -- | | 10,07 | 274 | 91 |
| Y | -- | | 10,07 | 280 | 92 |
| E | -- | | 4,25 | 290 | 93 |
| D | -- | | 3,65 | 298 | 94 |
| K | -- | | 10,53 | 301 | 95 |
| H | -- | | 6 | 305 | 96 |
| K | -- | | 10,53 | 306 | 97 |
| D | -- | | 3,65 | 307 | 98 |
| Y | -- | | 10,07 | 308 | 99 |
| K | -- | | 10,53 | 315 | 100 |
| R | -- | | 12,48 | 320 | 101 |
| Y | -- | | 10,07 | 325 | 102 |
| E | -- | | 4,25 | 328 | 103 |
| E | -- | | 4,25 | 330 | 104 |
| D | -- | | 3,65 | 335 | 105 |
| E | -- | | 4,25 | 344 | 106 |
| D | -- | | 3,65 | 348 | 107 |
| K | -- | | 10,53 | 349 | 108 |
| R | -- | | 12,48 | 354 | 109 |
| Y | -- | | 10,07 | 358 | 110 |
| D | -- | | 3,65 | 360 | 111 |
| H | -- | | 6 | 362 | 112 |
| R | -- | | 12,48 | 363 | 113 |
| H | -- | | 6 | 364 | 114 |
| R | -- | | 12,48 | 365 | 115 |
| Y | -- | | 10,07 | 370 | 116 |
| H | -- | | 6 | 372 | 117 |
| C | -- | | 8,18 | 377 | 118 |
| Y | -- | | 10,07 | 379 | 119 |
| R | -- | | 12,48 | 380 | 120 |
| R | -- | | 12,48 | 382 | 121 |
| Y | -- | | 10,07 | 386 | 122 |
| R | -- | | 12,48 | 388 | 123 |
| D | -- | | 3,65 | 389 | 124 |
| C | -- | | 8,18 | 393 | 125 |
| D | -- | | 3,65 | 396 | 126 |
| Y | -- | | 10,07 | 404 | 127 |
| Y | -- | | 10,07 | 405 | 128 |
| E | -- | | 4,25 | 413 | 129 |
| E | -- | | 4,25 | 420 | 130 |
| H | -- | | 6 | 421 | 131 |
| Y | -- | | 10,07 | 425 | 132 |
| E | -- | | 4,25 | 428 | 133 |
| R | -- | | 12,48 | 430 | 134 |
| R | -- | | 12,48 | 431 | 135 |
| D | -- | | 3,65 | 437 | 136 |
| D | -- | | 3,65 | 438 | 137 |
| R | -- | | 12,48 | 444 | 138 |
| Y | -- | | 10,07 | 447 | 139 |
| E | -- | | 4,25 | 453 | 140 |
| E | -- | | 4,25 | 454 | 141 |
| R | -- | | 12,48 | 456 | 142 |
| K | -- | | 10,53 | 457 | 143 |
| R | -- | | 12,48 | 458 | 144 |
| C | -- | | 8,18 | 460 | 145 |
| E | -- | | 4,25 | 461 | 146 |
| H | -- | | 6 | 466 | 147 |
| K | -- | | 10,53 | 468 | 148 |
| D | -- | | 3,65 | 469 | 149 |
| K | -- | | 10,53 | 476 | 150 |
| K | -- | | 10,53 | 477 | 151 |
| K | -- | | 10,53 | 480 | 152 |
| E | -- | | 4,25 | 484 | 153 |
| H | -- | | 6 | 486 | 154 |
| D | -- | | 3,65 | 488 | 155 |
| Y | -- | | 10,07 | 489 | 156 |
| H | -- | | 6 | 492 | 157 |
| D | -- | | 3,65 | 498 | 158 |
| K | -- | | 10,53 | 499 | 159 |
| Y | -- | | 10,07 | 500 | 160 |
| E | -- | | 4,25 | 503 | 161 |
| K | -- | | 10,53 | 504 | 162 |
| K | -- | | 10,53 | 506 | 163 |
| H | -- | | 6 | 510 | 164 |
| H | -- | | 6 | 518 | 165 |
| R | -- | | 12,48 | 522 | 166 |
| E | -- | | 4,25 | 523 | 167 |
| K | -- | | 10,53 | 524 | 168 |
| L | 2,36 | -- | | 527 | 169 |

1303.23........../169...........=**7,48983**............. Number of pKa 167....+2....=169........=NpK 1QQW

Are present four Cysteine residues $pK_{RR}$ =8.18; Sum of 169 pKa values in table 1303.23..........

Tasks for catalase molecule 1QQW.pdb

Protolytic constant $pK_a$ isoelectric point IEP=$pK_a$ calculate of side chains

$\Sigma pK_{aRside\ group}$ ; Nterminal $pK_{aNterminal}NH_3^+$ and $pK_{aCterminalCOO-}$constants

sum divide with number of acid groups $NpK_a$:

$IEP=pK_a=(\Sigma pKa_{Rside\ group}+pKa_{Nterminal}+pKa_{Cterminal})/NpKa$

Acid groups number in sum NpKa=167.......+2.........= 169.....

527 amino acids of them for $pK_a$ side groups number 167+2.

N-terminal Methionine M $pK_{aNterminal}$=9.21 and

C-terminal Lysine K $pKa_{Cterminal}$=2.34

Sum are calculate as

$\Sigma pKa=\Sigma pKa_{Rside\ group}+pK_{aNterminal}+pKa_{Cterminala}$=1303.23...........

**1.** Average constant $pK_{mean}=pK_a$=IEP **ISOELEKTRIC POINT**

NpKa=167.......+2........=169........

IEP=ΣpKa/ NpKa =1303.23/ 169 =**7,48983**.............

At pH value on isoelectric point pH**=IEP total charge** is zero „**0**"

zero charge „**0**" **IEP**=pH

**COOH** & **-$NH_3^+$** positive **$COO^-$** & **$NH_3^+$** negative **-$COO^-$** & **-$NH_2$**

<u>Underline</u> existing!

**2.** 1QQW molecule charge sign (**+**). zero „**0**" or (**-**) at pH=7.36

<u>Underline</u> existing:

**COOH**,**$NH_3^+$** <u>positive</u> + pH=7.36<IEP=**7,49** negative-**$COO^-$**,**$NH_2$**.

**3.** 1QQW molecule charge **+**. zero „**0**" or **-** at **electrophoresis** pH **8.8**

<u>Underline</u> existing:

**COOH**,**$NH_3^+$** positive +IEP=**7,49**<pH = **8,8** <u>negative</u> **-** **$COO^-$**,**$NH_2$**

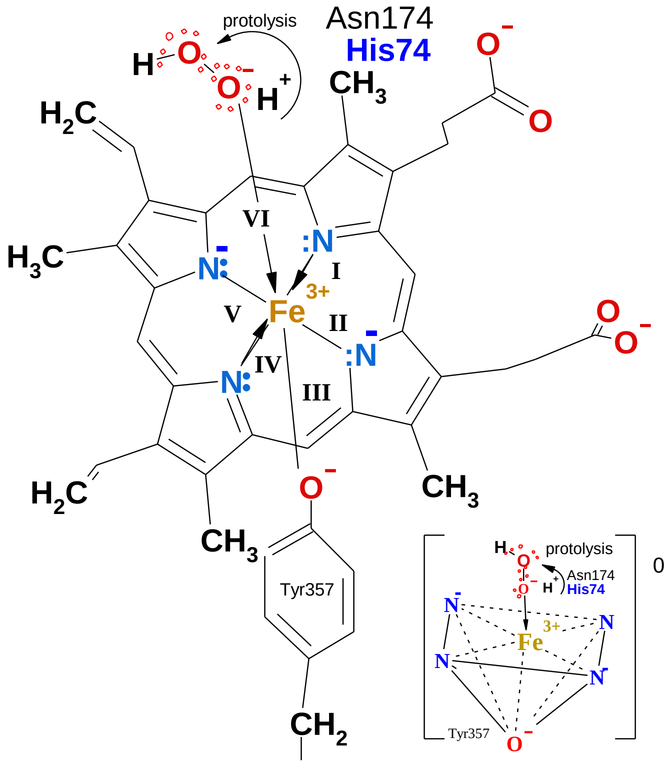
**4.** Calculate solution pH C=$10^{-7,23017}$ M 1QQW by *Ostwald dilution law*

concentration C in logarithm:

$$pH=\frac{pK_a-\log C}{2}=\frac{7{,}48983-\log 10^{-7{,}23017}}{2}=\frac{7{,}48983+7{,}23017}{2}=\mathbf{14{,}7201}/2=7{,}36......$$

Attractor 7,36 concentration of 1QQW is $10^{-7,23017}$..........M.

**5.** What secondary structures contains the CATALASE? .........**13 Alpha helixes** and .........**beta barrel 8 strands**.
**6.** What **alpha helices** constitute CATALASE polypeptide molecule? ........**13 Alpha-helices**
**7.** What **beta structure** and **sheets** and how many **beta strands** constitute CATALASE? .............**beta-barrel structure** with ...........................................**8 anti-parallel strands**.
**8.** What quaternary 4° structures components 3° subunits and what tertiary 3° structure domain units with its secondary 2° structures components are in given CATALASE unit?
.......4 four tetramer units of..........4 fourprotein chains; How many secondary 2° structures? ...........**13 Alpha-helices**; ............**beta-barrel structure** ...................**8 anti-parallel beta strands**.
**9**. **Funnel channel** long, wide, deep in angstrems distance?.....25.Å..........20-15 Å..........33-19Å
**10.** Wht are 11 **hydrophobic** **Funnel** AA numbers on polypeptide chain? **Val115**.....,**Ala116**...., **Pro128**....,**Phe152**....,**Phe153**....,**Phe163**....,**Ile164**....,**Pro178**.....,**Val181**....,**Leu198**.....,**Phe199**....
**11.** Wht are 14 **polar**-**charged** **Funnel** amino acids numbers on polypeptide chain ?!
......**Ser113**.......,**Glu118**........,**Ser121**........,**Arg126**........,**Asp127**........,**Gln167**........,**Lys168**......,
......**Lys176**.........,**Glu247**........,**His255**........,**Glu453**........,**Glu454**........,**Gln461**........,**His466**......
**12.** Whatare 31 amino acids numbers on polypeptide chain of Heme pocket tertiary 3° structure?
Val72....,Val73....,Ala75....,Val115.....,Ala116.......,Pro128.....,Gly130.....,Val145.....,
Gly146.....,Phe152.....,Phe153.....,Ile154.....,Ala157.....,Leu158.....,Leu159......,Phe160......,
Pro161....,Phe163......,Ile164......,Phe197......,Leu198......,Phe199......,Leu298....,Ala332.....,Phe333...,
Pro335......,Met349......,Leu350.......,Gly352.......,Phe355.........,Ala356.......,Pro358........,Ala434...
**13. Heme** pocket 8 **hydrophilic** amino acids numbers on polypeptide chain and 3 functions are?
...**Arg353**……,……..**Tyr**$^{357}$...........**Arg71**……,……**Arg111**……,……**Glu329**......,....**Arg364**.....
1) **His74,Asn147** catalysis ..................**H**$^{+}$ deprotonation for peroxide dismutation on **heme** iron
2) **H3=156-168 and H9=347-366** bind the ...........................................**heme** prosthetic group..
3) binding ....................................................**heme** propionic acid residues.
**14.** First Tertiary domain starting amino acid =....Asn3. and finishing amino acid=....Ala75..?
**15.** What two first alpha helices names are depicted? ...........**H1**..,..**H2**.......................................
**16.** Heme moiety domain starting amino acid =....Lys76. and finishing amino acid=....Asn320..?
**17.** 5 Helix names in **heme** domain:.....**H3**…,.....**H4**…..,.....**H5**…..,.......**H6**…..,......**H7**.....,
**18.** Beta sheet name and strands account: ....**beta-barrel and** ...............**8 anti-parallel strands**.
**19.** Third domain starting amino acid =........Pro321. and finishing amino acid= ........Asp436. ?
**20.** Carboxy terminal starting amino acid =..... Asp437. and finishing amino acid= ......Asn500.?
**21**. **Carboxy-terminal** globulin 4 Helix names:..**H10**.........,**H11**…......,..**H12**…......,..**H13**.............
**22**. How many polypeptide chains are linked to each heme? ..................one polypeptide chain..
**23.** What number of hems in biological unit of CATALASE **7cat.pdb**?..............four hemes.
**24.** What mass kD and number subunits make quaternary structure of CATALASE dumb-bell?..
.....four subunits, 60............kD each subunit molar mass, tetramer mass 60*4=.............240 kD.
**25**. **Heme** location distance from center the tetramer in angstroms is 45,66/2=22.83...........Å
**26.**How much **salt bridges** are present in tetramer?...28 bridges, Show **Arg**-**Asp**,**Glu** Functional groups interaction! **Arg**≡**C**— **N**$H_3^+$..........=>···**salt bridge**···<=.............$^{-}$**OOC** —**C**≡**Asp**,**Glu**..
**27. Heme** proximal components 6 and of α helix **H9** 3 amino acids numbers on polypeptide chain?
**Val**$^{145}$…..,**Pro**$^{335}$.....,**His**$^{217}$.....,**Arg**$^{353}$.....,**Ala**$^{356}$.....,**Tyr**$^{357}$......and **H9** **Arg**$^{353}$.....,**Ala**$^{356}$.....,**Tyr**$^{357}$......
**28. Heme** location, distal side structural components? distal side facing the........ channel contains .............non polar and .........polar residues, some of which are contributed by the beta-barrel..........
**29.** What five 5 intermolecular forces are known in biochemistry and physiology of proteins? ...
1.…**Hydrogen bond** 2.…**Hydrophobic** 3... **Salt bridges** 4.-**S**-**S**-…**disulfide bonds** 5.…**Coordinative bond**
**30.** What four **4** intermolecular forces fold protein chains of CATALASE? Call dentified!
1.…**Hydrogen bond** 2.…**Hydrophobic** 3... **Salt bridges** 5.…**Coordinative bond**
**31.** Describe the CATALASE **heme** pocket vicinity components: pyrrole rings, propionic




acid residues, hydrophobic pocket complex maker atom bonding properties are coordination number N=VI..............................................

**32.** Put in line six atoms which form coordinative bonds with ion $Fe^{3+}$! Iron!

**:N,:N⁻,:N⁻,:N⁻, –O⁻,** H-:•:O-:-O:•:-H..................

1 2 3 4 5 6....................

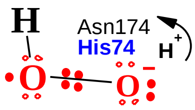
**33.** Do account coordination number **N=VI…** of iron **Fe** on center of given CATALASE Heme! Mark on left !

**34.** Which nonpolar, polar or ionic coordination bond of iron **Fe** belongs to –**O⁻** group of Tyr357? **Ionic bond**..............................

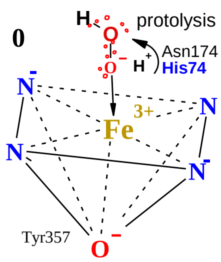
**35.** Explain Asn147,His74 role in CATALASE! Involved in proton **H⁺**... transfer ................................ to connect with the hydroxyl group **HO⁻+H⁺-Asn147**,His74.........................**->H₂O**

**36.** Show collision semi hexagonal, reverse piramidal coordination and give to coordinative complex neutral zero charge........................

**37.** Peroxide deprotonate **H:-•:O-::-O⁻::** +**H⁺** and explain anion free electron reactivity! Reactive mean radical with free ....... • electron anion with ........negative charge **HOO⁻**..........




**37.a** Show peroxide anion and iron **Fe(III)** collision small activation energy 29 $^{J}/_{mol}$ as negative attracts positive .......charge




**38.** What and how in complex reaction sequence favors and produce the **CATALASE**? .....................................

1) favors stabile efficiency • 100% product essential unsaturated fatty acids ω=6, ω=3.........................................

2) because erasing peroxide $\mathbf{H_2O_2}$ to zero $[\mathbf{H_2O_2}]^2$=.......... $^{mol}/_{liter}$..

3) **CATALASE** favors thirty million times 30•10⁶ production of life resources: ..................
and ethylene group **-CH₂-CH₂-** on dehydrogenation to cis ...........................

**39.** Reaction non catalytic spontaneous disproportionation. Protolysis create anions collision!

Protolysis $pK_a$=11,75: $2H_2O_2+2H_2O \rightarrow H_3O^+ + HOO^- + ^-OOH + H_3O^+$................create dismutation collision :

$2H_2O_2+2H_2O \rightarrow H_3O^+ + HOO^- >< ^-OOH + H_3O^+ \rightarrow$ $O_{2aqua}+4H_2O+Q_{exothermic}$...............................;

deprotonate anion oxygen collision products = **oxygen** + **water** + **heat** .

**40.** Write the dismutation reaction mechanism in steps with protonation **His74**, Asn174 of peroxide deprotonation in collisions with active site **Fe(III)-O**-Tyr357-**E**:

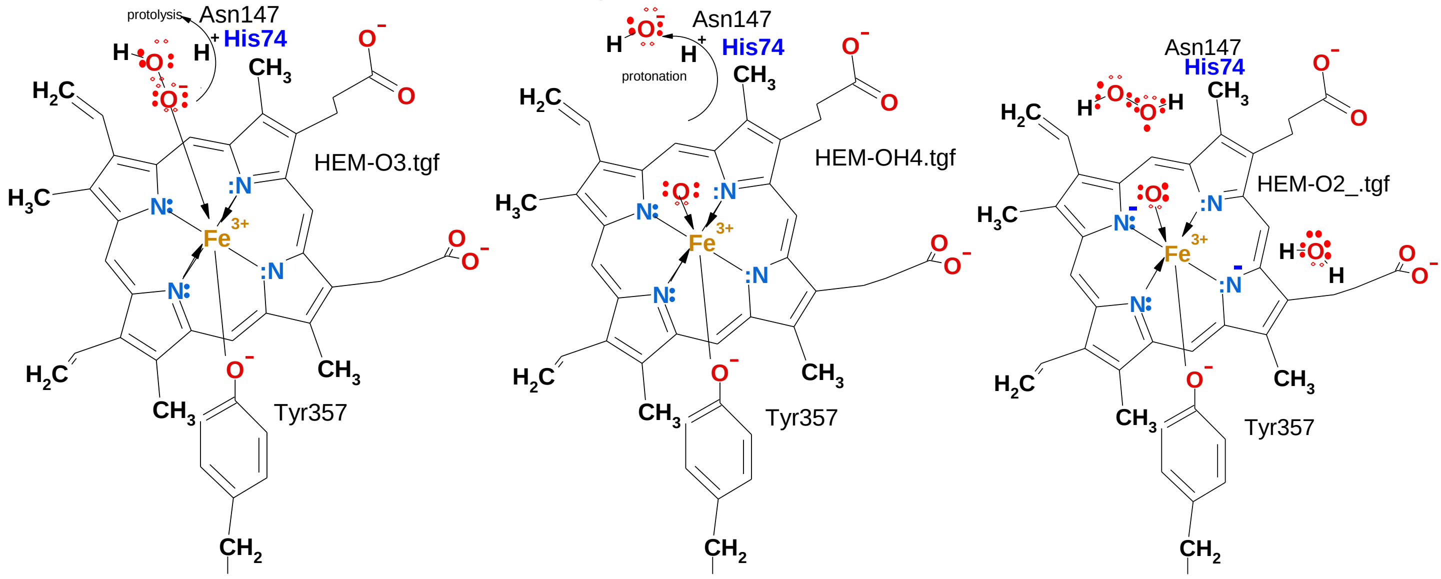
1. **H-O-O-H** $_{protolysis}$+**His74**+**Fe(III)-O**-Tyr357-**E**=>**H⁺-His74**$_{protonate}$+**HOO⁻**→+**Fe(III)-O**-Tyr357-**E** .............
2. **H⁺His74**$_{protonation}$+**HOO⁻**→+**Fe(III)-O**-Tyr357-**E**=>**HO⁻**$_{Red}$+**H⁺His74**$_{protonate}$+Ox**O-Fe(IV)-O**-Tyr357-**E**.......
3. **HO⁻**$_{Red}$+ **H⁺-His74**$_{protonate}$+Ox**O-Fe(IV)-O**-Tyr357-**E**=>$_{Red}$**H₂O**+**His74**+Ox**O-Fe(IV)-O**-Tyr357-**E** ...............
4. =>**H-O-O-H** $_{protolysis}$+Asn147+**O-Fe(IV)-O**-Tyr357-**E** =>**H⁺**Asn147+**HOO⁻**→+**O-Fe(IV)-O**-Tyr357-**E** ...........
5. **H⁺**Asn147+**HOO⁻**→+**O-Fe(IV)-O**-Tyr357-**E**=>**HO⁻**$_{Red}$+**H⁺**Asn147+Ox**O-O-Fe(IV)-O**-Tyr357-**E**.................
6. =>**HO⁻**$_{Red}$+**H⁺**Asn147+Ox**O-O-Fe(IV)-O**-Tyr357-**E**=>$_{Red}$**H₂O**+Asn147+Ox**O-O-Fe(IV)-O**-Tyr357-**E** ..........
7. $_{Red}$**H₂O**+Ox**O-O-Fe(IV)-O**-Tyr357-**E**=>$_{Red}$**H₂O**+Ox**O=O**+-**Fe(III)-O**-Tyr357-**E** ............................

Summary: $2H_2O_2$+**CAT**→$H_3O^+$+**HOO⁻**>**Fe(III)**<⁻**OOH**+$H_3O^+$→$O_{2aqua}+2H_2O+Q_{exothermic}$+**CAT**

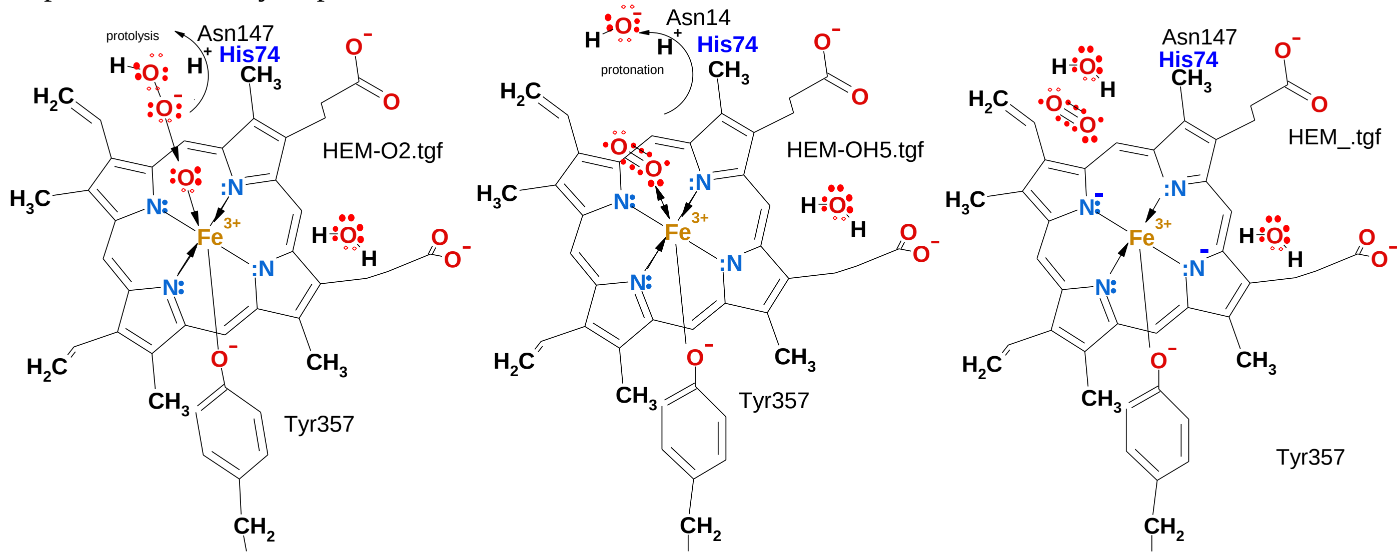
Protolysis activate transition state complex **oxygen**+ **water**+ **heat**+ CATALASE,

1. Colliding oxygen atom oxidized Ox **O-Fe(III)** and deprotonate on **H⁺ His74**, Asn174;........
2. second oxygen atom reduced **HO⁻**Red and protonated neutral about **H₂O**............

**41.** What is happen with CATALASE during life resources production $O_2+H_2O+Q$?




Hem pocket with 28 hydrophobic amino acids – in <u>waterless</u> medium oxidation-reduction reaction absent:




**42.** For what reason CATALASE is tightly bound to **NADPH**?

Tyr357-**OH**+$Fe^{2+}$+**NADP$^+$**+**$H_2O$**($H^+$-His161)⇔Tyr357-**$O^-$**+$Fe^{4+}$+**NADPH**+**$H_3O^+$**+(His161)

**NADPH** stabilizing Tyr357-**$O^-$** + $Fe^{3+}$ionic bond ............................shifts equilibrium to right

with high rate protolysis attractors pH=7,36...... and concentration [$H_2O$]=55,3.......$^{mol}/_L$

**43.** Two beta sheets Intermolecular hydrogen bonds connecting in tetramer subunits with 4 beta strands.......................................................................................... 1st <u>page</u>:

**44.** Show Hydrogen <u>bond</u> between electronegative element atoms **O** and **N** peptide bond carbonyl >**C=O** and imino group hydrogen >**C=O…H—N**<..............................

and imino group hydrogen >**N—H** and carbonyl group >**N—H**...**O**=**C**<.........................

or between carbonyl >**C**=**O** and hydroxyl Ser hydrogen, amino residues >**C**=**O**...**H—O**—Ser....

or between carbonyl >**C**=**O** and amino hydrogen His residue >**C**=**O**..**H—N**<His.............

**45.** Arrhenius velocity constant **k**→ expression active collision number $e^{-Ea/(RT)}$=**exp(-E$_a$/(RT))**=0.988......!

$\vec{k}$ = **A**....•$e^{-Ea/(RT)}$................

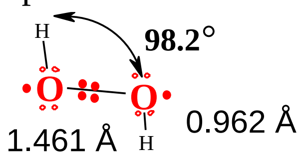
activation energy $E_a$,= 29...... $^J/_{mol}$ **;**
geometric factor **A=0,13** ...... and
the temperature **T=298,15** ..... K.

**46.** How many times decreases activation energy $\mathbf{E_a}$ for CATALASE to compare absence catalyst?
$\mathbf{E_{aCATALASE}}$ =29 J/mol; ..........................$\mathbf{E_{a(absence\ catalyst)}}$ =79000 J/mol
79000/29=2724 ..................................times smaller $\mathbf{E_a}$ for CATALASE.
**47.** How many times increases pre exponential - geometric factor for CATALASE?
.$\mathbf{A_{absence\ catalyst}=0.01}$............................., $\mathbf{A_{CATALASE}=0.13}$ ......................................and
**0.13/0.01=13**................................ **times** improve pre exponential - geometric factor $\mathbf{A_{CATALASE}}$.

**48.** What physical meaning has Boltzmann exponential factor value 0.988 = $\mathbf{exp(-E_a/(RT))}$?

$$\vec{\mathbf{k}} = \mathbf{A}\bullet \mathbf{e}^{-\frac{\mathbf{Ea}}{\mathbf{RT}}} = \mathbf{A}\bullet 0.988$$

Correct performed collision number is 988 of total 1000.
....
**49.** What physical meaning has pre exponential-geometric factor 1=**A**?
Perfect geometry of peroxide molecules for collision is **A**=1...
as from 100 total collisions correct collision number is 100.................
**50.** What physical meaning has perfect pre exponential-geometric factor?
fraction perfect is 1 as mean 100% .......................perfect collisions .




**51.** Measure the geometry of peroxide bond angle, distance between **O** – **H** and **O - O** put in text boxes of structure!
**52.** What many times increases CATALASE velocity constant for 1 mol in liter $\mathbf{H_2O_2}$ conversion to life resources $\mathbf{O_2+H_2O+Q}$? **oxygen**+**water**+**heat** + CATALASE?

$$\sqrt{\vec{\mathbf{v}}} = {}^{\mathbf{CAT}}\sqrt{\vec{\mathbf{k}}}\ \bullet[\mathbf{H_2O_2}] = \mathbf{0.36}\bullet[\mathbf{H_2O_2}];\ .......$$

$$.......\ {}^{\mathbf{CAT}}\sqrt{\vec{\mathbf{k}}}\ /\ \sqrt{\vec{k}} = 0{,}36/1{,}19\bullet 10^{-8} = 30\bullet 10^{6}\ .......$$ times greater velocity constant.

Solubility, protolytic dismutation has compensation for the participation of water $2H_2O_{2aq}+2H_2O=O_{2aq}+3H_2O$.

Half-reaction: Ox $H_2O_2+2H_2O=O_{2gas}+2H_3O^++2e^-$; **absolute** standard potential for gas $O_{2agas}$ $E^\circ_{H2O2}=0.5268$ V;
Ox $H_2O_2+H_2O=O_{2aqua}+2H_3O^++2e^-$; **Absolute** standard potential in $O_{2aqua}$ aqueous solution $E^\circ_{OxH2O2}=0.4753$ V;
Red $H_2O_2+2\ H_3O^++2\ e^-=4\ H_2O$ ; **Absolute** inverse standard potential of reduction $-E^\circ_{RedH2O2}=-1.7113$ V.

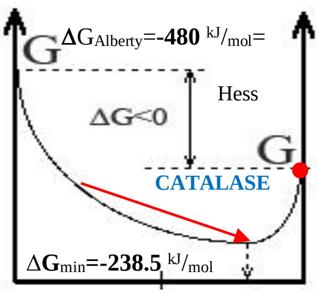
| *Viela* | $\Delta H^\circ_H$ kJ/mol | $\Delta S^\circ_H$ J/mol/K | $\Delta G^\circ_H$ kJ/mol | Solubility, protolysis dismutate peroxide $2H_2O_{2aq}+2H_2O=O_{2aq}+3H_2O$; |
|---|---|---|---|---|
| $H_3O^+$ | -285.81 | -3.854 | -213.275 | $\Delta G^\circ_{H3O^+}$, kJ/mol Mischenko 1972, Himia, Leningrad [26] |
| $H_2O_{2aq}$ | **-191.99** | **-481.688** | **-48.39** | **BiochemThermodynamic 2006** Masachusets Technology Institute |
| $H_2O_{2aq}$ | -191.17 | 143.9 | -134.03 | University Alberta 1997. |
| $H_2O_{2aq}$ | Formation | **-48.39** | **340.25** | $G_{H2O2aq}=\Delta G_{H2O2Alberty}+(G_{O2gas}+G_{H2gas})=$**340.25** kJ/mol; |
| $H_2O_{2aq}$ | Formation | -134.03 | **254.61** | $G_{H2O2aq}=\Delta G_{H2O2Alberty}+(G_{O2gas}+G_{H2gas})=$**254.61** kJ/mol; |
| $H_2O_{2aq}$ | Formation | **-148.985** | **284.255** | $G_{H2O2aq}=\Delta G_{H2O2form}+(G_{O2gas}+G_{H2gas})=$**284.255** kJ/mol; |
| $H_2O_{2aq}$ | $\Delta E^\circ_{H2O2aq}=$ | **1.236 V** | **284.255** | $G_{AlbertyH2O2}=(G_{O2Biochem}+G_{H2O}-\Delta G_{eqBioChem})/2=$**284.255** kJ/mol; |
| $HOO^-$ | $pK_a=11.75$ | **77.016** | **338.831** | $G_{HOO^-}=-G_{H3O^+}+\Delta G_{aH2O2}+(G_{H2O2}+G_{H2O})=$**338.831** kJ/mol; |
| $O_{2aa}$ | **-11.70** | **-94.2** | **16.40** | pH=7.36 [8] Biochem. Thermodyn Massachusetts Technology Inst. |
| $O_{2aq}$ | -11.715 | 110.876 | 16.4 | CRC [1] $G_{O2aqua}=$**330** kJ/mol; [14,15] |
| $H_2O$ | **-286.65** | **-453.188** | **-151.549** | pH=7.36 [8] Biochem. Thermodyn Massachusetts Technology Inst. |
| $H_2O$ | -285.85 | 69.9565 | -237.191 | CRC [1] $G_{H2O}=$**0** kJ/mol; [14,15] |

**Absolute** potential **scale 0.4753** Volts and **-1.7113** Volts obtained result $\Delta G_{eqStandart\_H2O2}=$**-238.51**....... kJ/mol:
$\Delta G_{eqStandard\_H2O2}=(E^\circ_{OxH2O2}-E^\circ_{RedH2O2})*F*n=(0.4753-1.7113)*96485*2=(-1.236)*96485*2=-238.51$ kJ/mol
coincides with the **Alberty absolute** free energy **scale** in the Hess calculation: $\Delta G_{eqStandard}=$**-238.51**....... kJ/mol :
Calculation of Hessian free energy change $\Delta G_{eqStandard}=G_{O2aqua}+G_{H2O}-2*G_{H2O2}=$**330+0-2*284.255=-238.51** kJ/mol;
$G_{H2O2}=(G_{O2aqua}+2*G_{H2O}+\Delta G_{Alberty\_2H2O2})/2=$(**330+2*0+238.51**)/2=**568.51**/2=**284.255** kJ/mol ;
The **absolute** potential **scale** coincides with the **Alberty absolute** free energy **scale.**

$$K_{eqStandard}=\frac{[O_2]_{aqua}\cdot[H_2O]}{[H_2O_2]^2_{aqua}}=\exp(-\Delta G_{eqStandard}/R/T)=\exp(228573/8.3144/298.15)=6.11*10^{41}........=10^{41.8}$$

$[H_2O_2]$=1M; biochemistry concentrations $[O_{2aqua}]=6*10^{-5}$ M, $[H_3O^+]=10^{-7.36}$ M, $[H_2O]$=55.3 M.
$E_{Red}=E^\circ_{H2O2}+0.0591/2\bullet lg([O_{2aqua}]*[H_3O^+]^2/[H_2O_2]/[H_2O])=$**0.4753**$+0.0591/2*lg(6*10^{\wedge(-5)}*10^{\wedge(-7.36*2)}/1/55.3)=$**-0.13593** V
$E_{Ox}=-E^\circ_{H2O2Ox}+0.0591/2\bullet log([H_2O_2]*[H_3O^+]^2/[H_2O]^4)=$**-1.7113**$+0.0591/2*lg(1*10^{\wedge(-7.36*2)}/55.3^{\wedge4})=$**-2.3523** V
$[H_2O_2]$=1 M; $\Delta G_{eqBioChem}=(E_{Red}+E_{Ox})*F*n=$(**-0.13593-2.3523**)*96485*2=(**-2.48823**)*96485*2=**-480.15** kJ/mol ;
$\Delta G_{Alberty}=G_{O2Biochem\_arterial}+G_{H2OBioChemistry}-2*G_{H2O2}=$**88.22+85.64-2*284.255=-394.65** kJ/mol;
Biochemistry concentrations $[H_2O_2]=10^{\wedge(-10)}$ M, $[O_{2aqua}]=6*10^{-5}$ M, $[H_3O^+]=10^{-7.36}$ M, $[H_2O]$=55.3 M
$E_{Red}=E^\circ_{H2O2}+0.0591/2\bullet lg([O_{2aqua}]*[H_3O^+]^2/[H_2O_2]/[H_2O])=$**0.4753**$+0.0591/2*lg(6*10^{\wedge(-5)}*10^{\wedge(-7.36*2)}/10^{-10}/55.3)=$**0.15957** V
$E_{Ox}=-E^\circ_{H2O2Ox}+0.0591/2\bullet log([H_2O_2]*[H_3O^+]^2/[H_2O]^4)=$**-1.7113**$+0.0591/2*lg(10^{\wedge(-10)}*10^{\wedge(-7.36*2)}/55.3^{\wedge4})=$**-2.64777** V
$\Delta G_{eqBioChem}=(E_{Red}+E_{Ox})*F*n=$(**0.15957-2.64777**)*96485*2=(**-2.4882**)*96485*2=**-480.15** kJ/mol
$\Delta G_{Alberty}=G_{O2Biochem\_arterial}+G_{H2OBioChemistry}-2*G_{H2O2}=$**88.22+85.64-2*284.255=-394.65** kJ/mol. The **absolute** potential **scale** coincides with the Alberty **absolute** free energy **scale** at all concentrations $10^{\wedge(-10)}$ M <$[H_2O_2]$<1 M.

The free energy change of the exothermic and exoergic $H_2O_{2\ (aq)}$ dismutation Homeostasis reaction is $\Delta G_{eqBioChem}=$**-480**..........kJ/mol negative. The Hess **Alberty** free energy change $\Delta G_{HessAlberty}=$**-238.5**........kJ/ mol is negative too. The **absolute** potential scale $\Delta G_{eqStandart\_H2O2}=$**-238.5**..........kJ/mol coincides with the **absolute** scale for free energy. When reaching the mixture constant $K_{eqStandart}=10^{41.8}$..... equilibrium state is the occurrence of the minimum $\Delta G_{min}$ of the free energy change so called the Prigogine attractor. High-speed protolysis attractors pH=7.36, oxygen in the air 20.95% are in equilibrium, while homeostasis continues irreversibly, because is a non-equilibrium state there. Prigogine attractor Nobel Prize in Chemistry in 1977.
CATALASE quenches peroxide molecules $H_2O_2$ for one hundred percent ω=6, ω=3 yield for the synthesis of essential fatty acids C20:4 elongation in peroxisomes. The reactivity of CATALASE is an irreversible homeostasis indispensible Brownian molecular engine for evolution and survival.




**A+A 50% B+2C.**

**reactants** $2H_2O_{2(aq)}$

**products** $O_{2aqua}+2H_2O$

Conclusions

$H_2O_2+H_2O_2+Fe^{3+} \rightarrow H^++HOO^->Fe^{3+}<^-OOH+H^+ \rightarrow O_{2aqua}+H_2O+H_2O+Q_{exothermic}+Fe^{3+}$.
Protolysis activate transition state active complex **oxygen**+**water**+**heat** +CATALASE
CATALASE reactivity producing life resources $O_{2aqua}+2H_2O+Q$

**54.**1. **Catalyst** CATALASE (CAT) is involved to reaction active transition state complex formation : **$H_2O_2$…CAT…$H_2O_2$** and on finish released into products free unchanged CAT. ..........

**54.**2. **Catalyst** CAT decrease activation energy $E_a$ from 79000 J/mol to 29 J/mol times 2724 less.

**54.**3. **Catalyst** CAT improve geometric factor A=0.01 to A=0.13 times 13 better. ..........

**54.**4. **Catalyst** CATALASE increase reaction velocity constant $\vec{k}$ from $1.9\bullet10^{-8}$ $M^{-1}s^{-1}$ to 0.36 $M^{-1}s^{-1}$ times $30\bullet10^6$ thirty million more. ..........

**54.**5. Prigogine attractor CATALASE reactivity is indispensable life molecular engine converting processes to ● 100% efficiency with erasing peroxide molecules.

**54.6.** CATALASE reactivity produces the life resources:
ω=6, ω=3 fatty acids **oxygen**+**water**+**heat**; $O_{2aqua}+2H_2O+Q$.................

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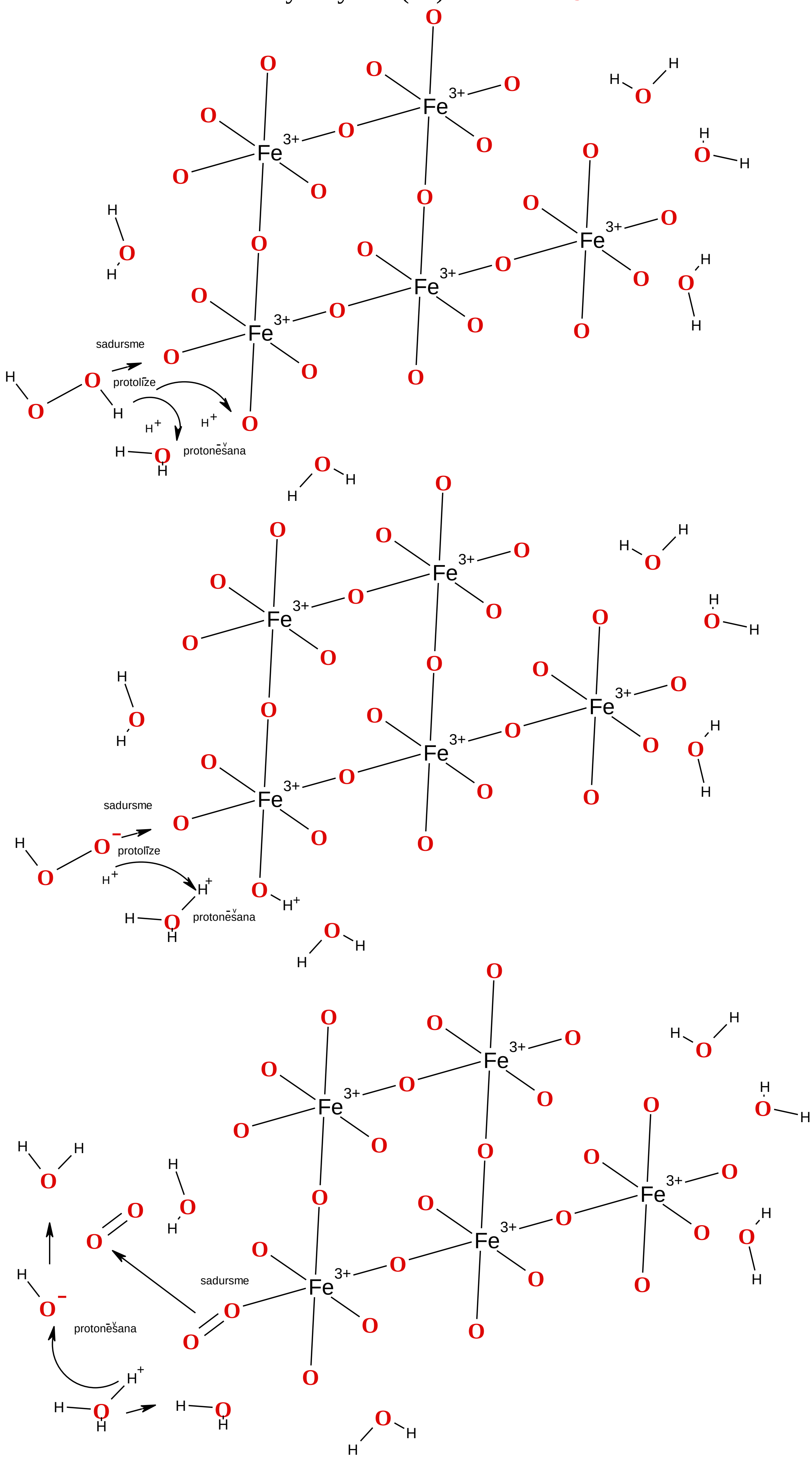
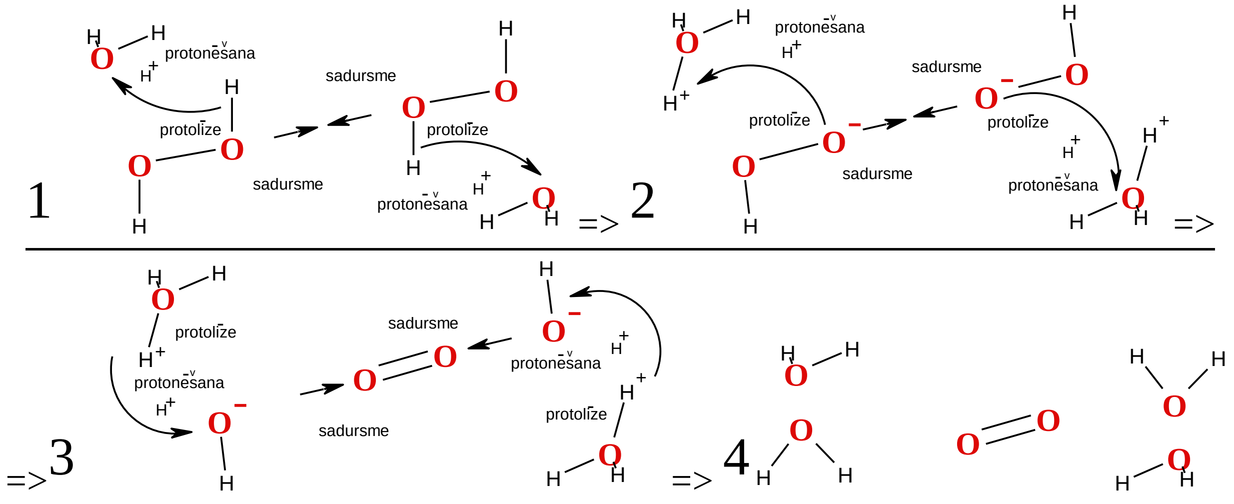
# Catalyst by iron(III) oxide $Fe_2O_3$.



$H_2O + H_2OO + OOH + H_2O \rightarrow H_3O^+ + HOO^- >< ^-OOH + H_3O^+ \rightarrow O_{2aqua} + 2H_2O + 2H_2O + Q_{exothermic}$




$H_2O_2 + H_2O_2 + CAT \rightarrow H^+ + HOO^- > CAT < ^-OOH + H^+ \rightarrow O_{2aqua} + H_2O + H_2O + Q_{exothermic} + CAT$

Catalyst by manganese(II) oxide MnO.