Electronic supporting information

Iron Phthalocyanine Modified Mesoporous Titania Nanoparticles for Photocatalytic Activity and CO₂ Capture Applications

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Figure-S1: Photolytic degradation of sulphur mustard in the absence of any catalyst under sunlight exposure.
Figure-S2: GC-MS spectra of SM & degradation products in sunlight on TiO$_2$ nano catalysts

- a- chloroethylvinyl sulfide,
- b- chloroethyl vinyl sulfoxide,
- c- bis(2-chloroethyl) sulfide,
- d- 2-chloroethyl 2-hydroxyethyl sulfide,
- e- bis(2-chloroethyl) disulfide,
- f- 2-chloroethyl 2-hydroxyethyl disulfide,
- g- bis(2-chloroethyl) sulfoxide,
- h- bis(2-chloroethyl) sulfone
Figure-S3: GC-MS spectra of SM & SM disulfide on Fepe-TiO$_2$ w.r.t time
Figure-S4: GC-MS spectra of SM & SM disulfide on nano TiO$_2$ w.r.t time
**Figure-S5:** Mass spectrum of SM sulfoxide

Name: Bis(β-chloroethyl) sulfoxide (Bis(2-chloroethyl) sulfoxide)  
Formula: C₄H₈Cl₂OS  
MW: 174  
CAS#: 5819-08-9  
NIST#: 273377  
ID#: 27668  
DBs: mainlib, RTECS, NIH  
Contributor: A.A.Kutin, Moscow, Russia  

10 largest peaks:  
63 999 | 27 894 | 76 407 | 65 274 | 47 121 | 59 118 | 45 111 | 26 108 | 112 97 | 83 80
Figure-S6: Mass spectrum of SM disulfide

Name: Disulfide, bis(2-chloroethyl) (Bis(2-chloroethyl) disulfide)
Formula: C4H8Cl2S2
MW: 190 CAS#: 1002-41-1 NIST#: 273398 ID#: 6901 DB: replib
Other DBs: None
Contributor: A.A. Katin, Moscow, Russia

10 largest peaks:
- 63 999
- 190 649
- 192 469
- 27 427
- 65 334
- 64 320
- 128 307
- 92 258
- 36 208
- 59 180
Figure-S7: Mass spectrum of Hemi sulphur mustard

Name: Ethanol, 2-(2-chloro-ethylthio)- (Hemisulfur mustard)
Formula: C₄H₉ClOS
MW: 140 CAS#: 693-30-1 NIST#: 226653 ID#: 3706 DB: replib
Other DBs: RTECS, NIH
Contributor: Dennis Rohrbaugh, CBDCOM/ERDEC, Edgewood, MD

10 largest peaks:

<table>
<thead>
<tr>
<th>Peak</th>
<th>abundance</th>
</tr>
</thead>
<tbody>
<tr>
<td>45 999</td>
<td>25 170</td>
</tr>
<tr>
<td>61 908</td>
<td>22 778</td>
</tr>
<tr>
<td>47 749</td>
<td>19 257</td>
</tr>
<tr>
<td>109 735</td>
<td>18 062</td>
</tr>
<tr>
<td>63 662</td>
<td>15 987</td>
</tr>
<tr>
<td>60 506</td>
<td>14 631</td>
</tr>
<tr>
<td>44 417</td>
<td>12 942</td>
</tr>
<tr>
<td>46 392</td>
<td>10 577</td>
</tr>
<tr>
<td>91 325</td>
<td>9 081</td>
</tr>
<tr>
<td>59 321</td>
<td>8 563</td>
</tr>
</tbody>
</table>
Figure-S8: Mass spectrum of chloro ethyl vinyl sulfoxide

Formula: C₄H₇ClO₅ (Vinyl 2-chloroethyl sulfoxide)
MW: 138 CAS#: 40709-82-8 NIST#: 226796 ID#: 39665 DB: mainlib
Other DBs: RTECS
Contributor: Dennis Rohrbaugh, CBDCOM/ERDEC, Edgewood, MD
10 largest peaks:
66 999 | 63 881 | 138 369 | 65 241 | 58 193 |
59 193 | 75 146 | 140 142 | 47 132 | 73 115 |
**Figure-S9**: Mass spectrum of 2-(2-Chloro-ethyl)disulfanyl)-ethanol

- **Name**: Ethanol, 2-[(2-chloroethyl)dithio]- 2-[(2-Chloroethyl)disulfanyl]ethanol
- **Formula**: C₄H₉ClOS₂
- **MW**: 172
- **CAS#**: 79503-74-5
- **NIST#**: 226639
- **ID#**: 3690
- **DB**: replib
- **Other DBs**: None
- **Contributor**: Dennis Rohrbaugh, CBDCOM/ERDEC, Edgewood, MD
- **10 largest peaks**:
  - 45 999 | 59 236 | 60 212 | 79 181 | 63 171 |
  - 47 140 | 43 135 | 46 124 | 92 117 | 64 109 |
Figure-S10: Mechanism of photocatalytic degradation of sulphur mustard.
### Table S1: Toxicity of degraded materials

<table>
<thead>
<tr>
<th>S. N.</th>
<th>Degraded Product</th>
<th>LD&lt;sub&gt;50&lt;/sub&gt; (mg/Kg)</th>
<th>LD&lt;sub&gt;L0&lt;/sub&gt; (mg/Kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Sulfur Mustard (SM)</td>
<td>mouse sc 125 iv 8.6</td>
<td>(b)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>human oral 0.7 skin 20</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>SM sulfoxide</td>
<td>NA</td>
<td>150 (b)</td>
</tr>
<tr>
<td>3</td>
<td>SM disulfide</td>
<td>NA</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>Chloroethylvinyl sulfide</td>
<td>NA</td>
<td>100 (b)</td>
</tr>
<tr>
<td>5</td>
<td>Chloroethylvinyl sulfoxide</td>
<td>NA</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>Thiodiglycol</td>
<td>Rat: oral, 6,610 mg/kg</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Guinea pig: oral, 3,960 mg/kg</td>
<td>(a)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Rabbit: skin, 20 ml/kg</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>Hemi sulfur mustard</td>
<td>Rat: im, 500 pg/kg</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Mouse: skin, 600 mg/kg</td>
<td>(a)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Mouse: 35 mg/kg</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>SM Sulfone</td>
<td>Rat: &gt; 72 mg/kg</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Mouse: 50 mg/kg</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Rat: sc, 50 mg/kg</td>
<td>(a)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Mouse: sc, 35 mg/kg</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>Divinyl sulfide</td>
<td>Rat: oral, 170 mg/kg</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Mouse: oral, 112 mg/kg</td>
<td>(a)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Rat: inhalation, 660 mg/m3</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Mouse: inhalation, 510 mg/m3</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>Hydroxy ethylvinyl sulfoxide</td>
<td>Nontoxic</td>
<td></td>
</tr>
</tbody>
</table>

LD<sub>50</sub> = median lethal dose; LD<sub>L0</sub> = lowest lethal dose; ip = intraperitoneal; iv = intravenous; sc = subcutaneous; NA-Not available

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**References**
