Electronic supporting information

Iron Phthalocyanine Modified Mesoporous Titania Nanoparticles for Photocatalytic Activity and CO_2 Capture Applications

P.V.R.K. Ramacharyulu[a], Raeesh Muhammad[a], J. Praveen kumar[b], G. K. Prasad[b*],

Paritosh Mohanty[a*]

[a]Department of Applied science & engineering, IIT Roorkee, Saharanpur-247001 (U.P.), India

[b]Defence R & D Establishment, Jhansi Road, Gwalior-474002 (M.P.), India

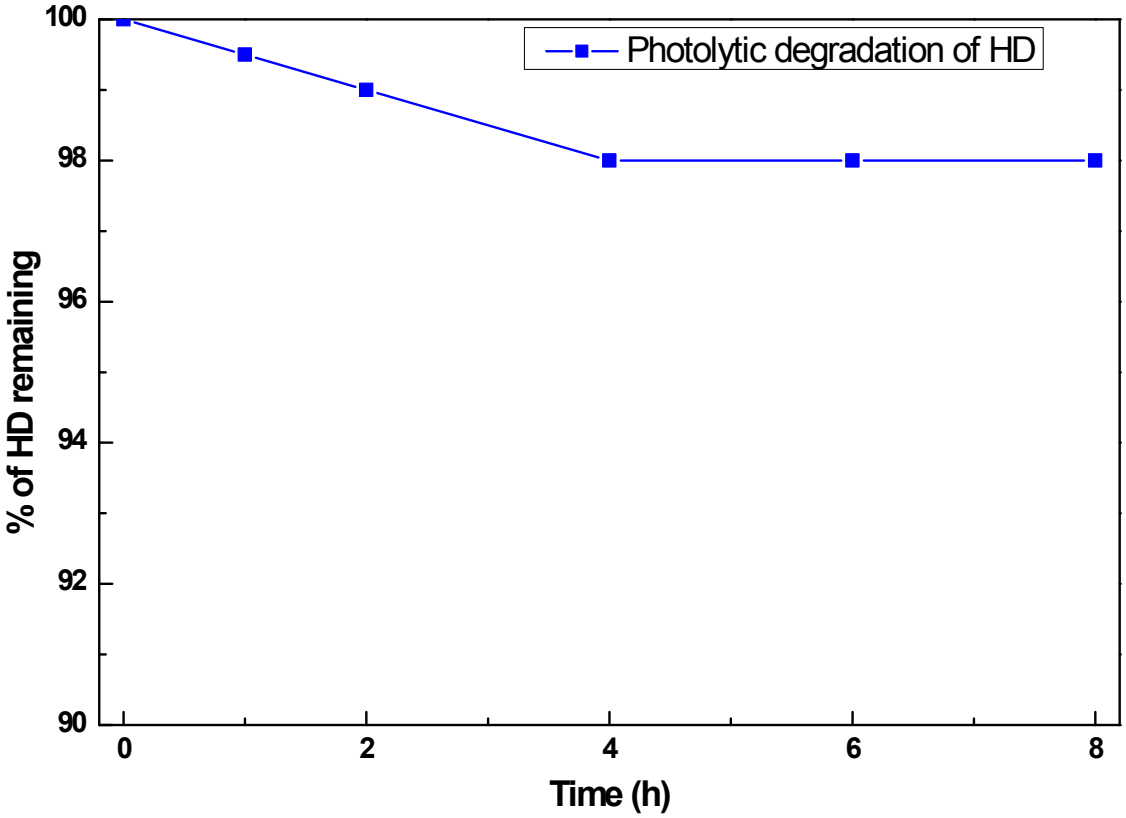
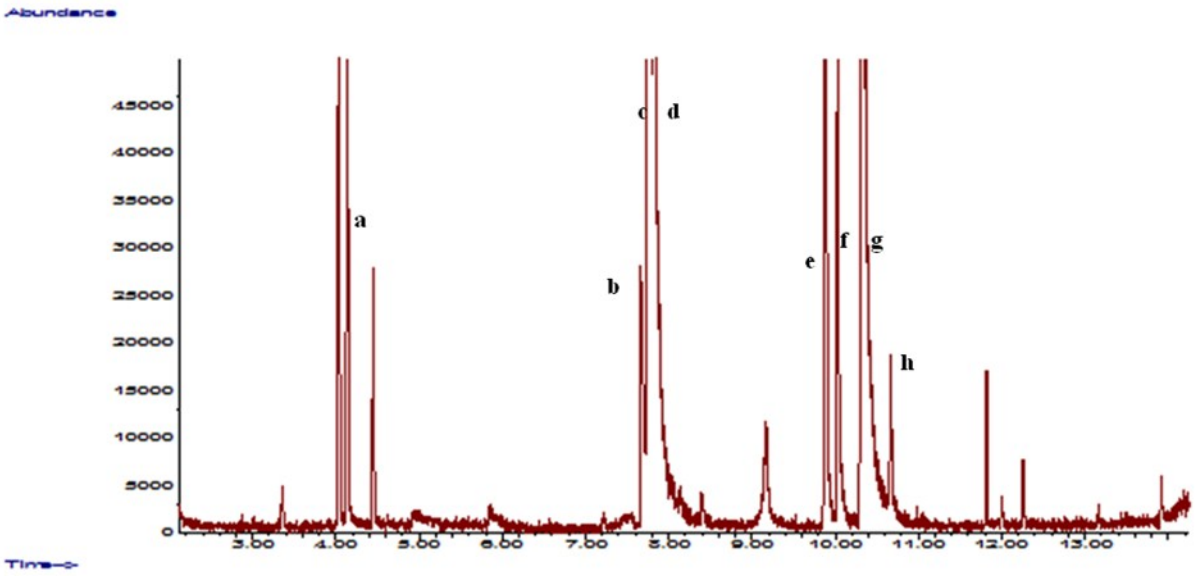


Figure-S1: Photolytic degradation of sulphur mustard in the absence of any catalyst under sunlight exposure.



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-S2: GC-MS spectra of SM & degradation products in sunlight on TiO_2 nano catalysts

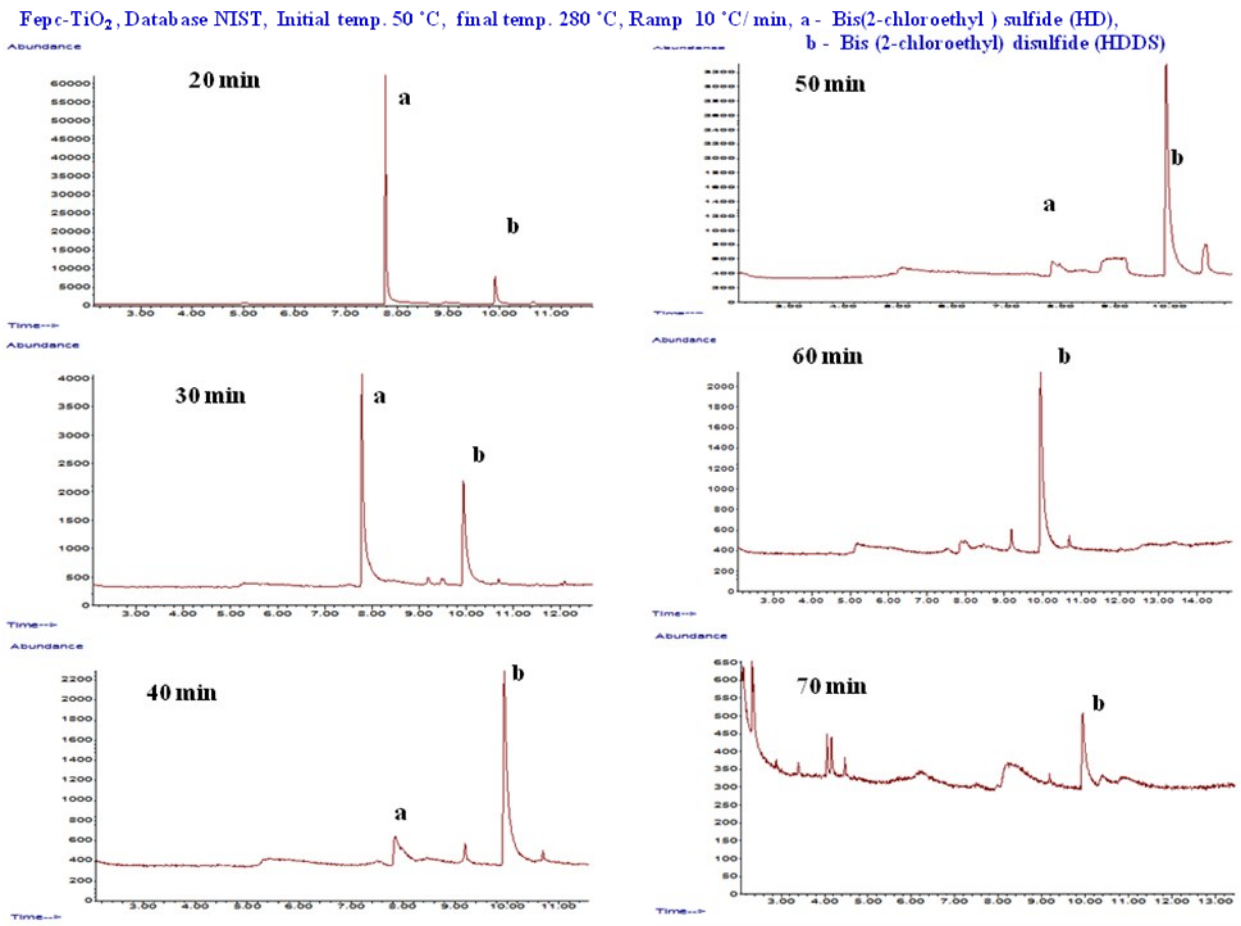


Figure-S3: GC-MS spectra of SM & SM disulfide on Fepc-TiO_2 w.r.t time

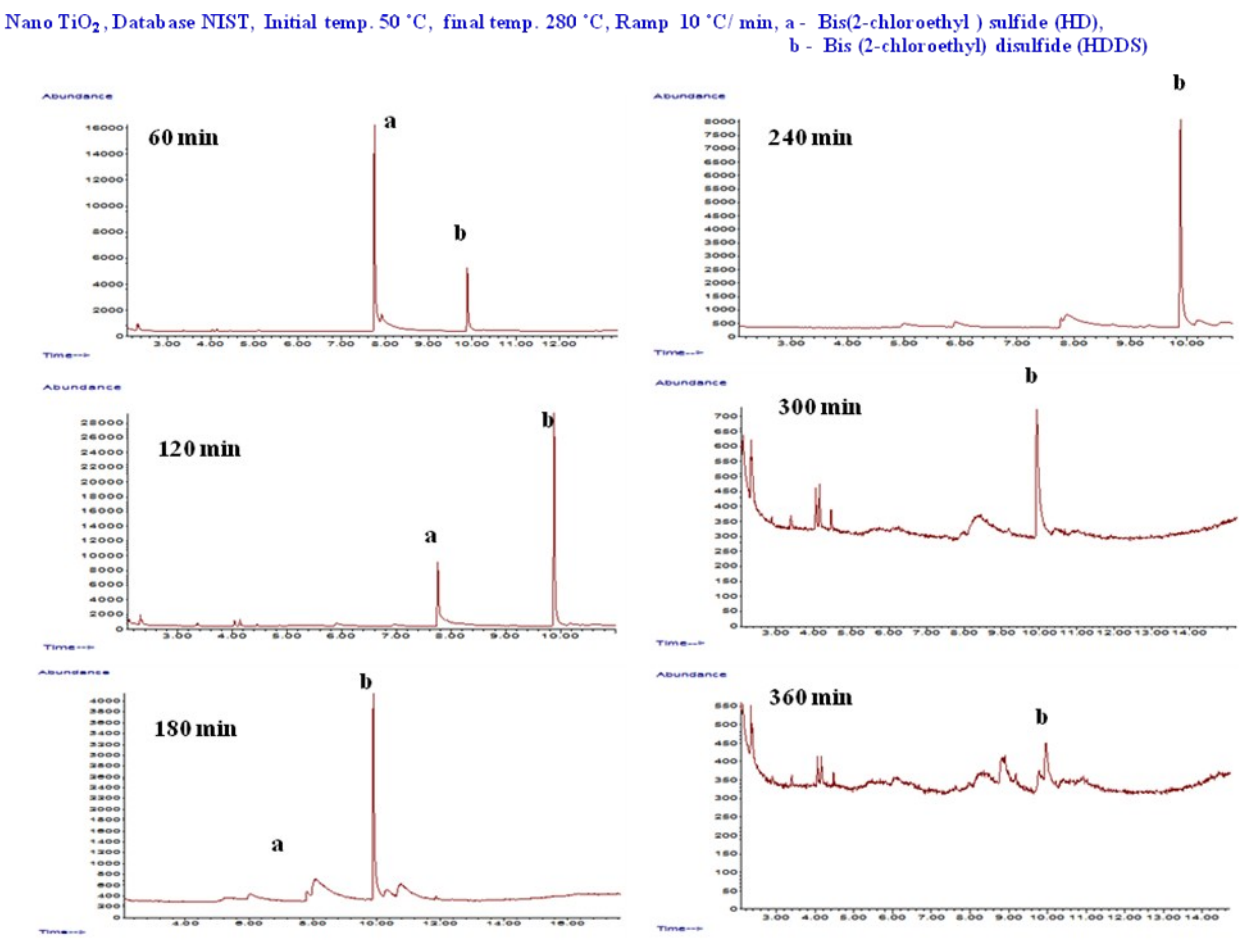


Figure-S4: GC-MS spectra of SM & SM disulfide on nano TiO_2 w.r.t time

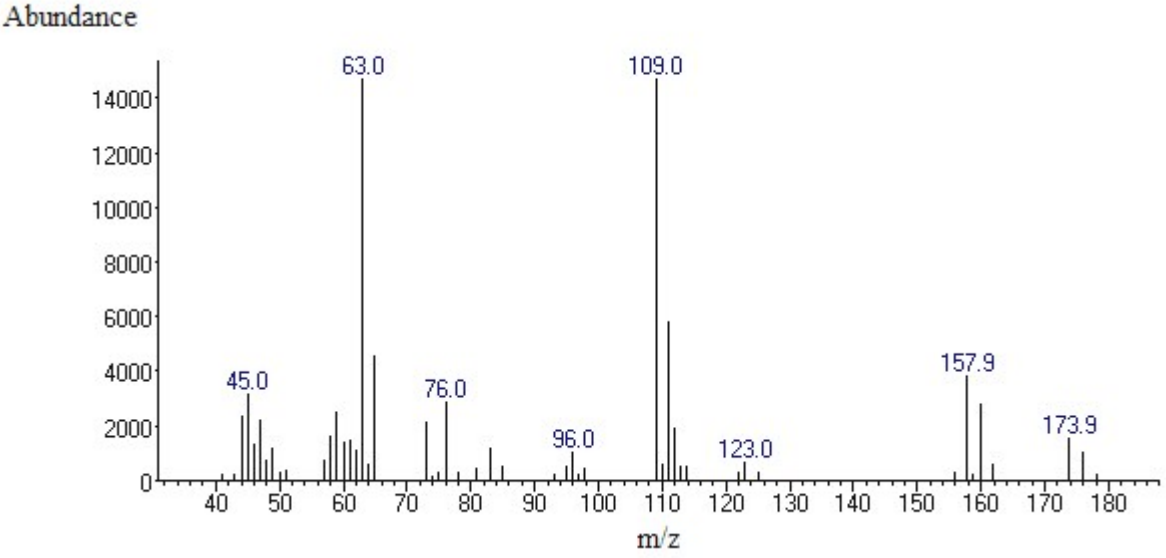


Figure-S5: Mass spectrum of SM sulfoxide

Name: Bis(β-chloroethyl) sulfoxide (Bis(2-chloroethyl) sulfoxide)
Formula: $C_4H_8Cl_2OS$
MW: 174 CAS#: 5819-08-9 NIST#: 273377 ID#: 27668 DB: mainlib
Other DBs: 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 |

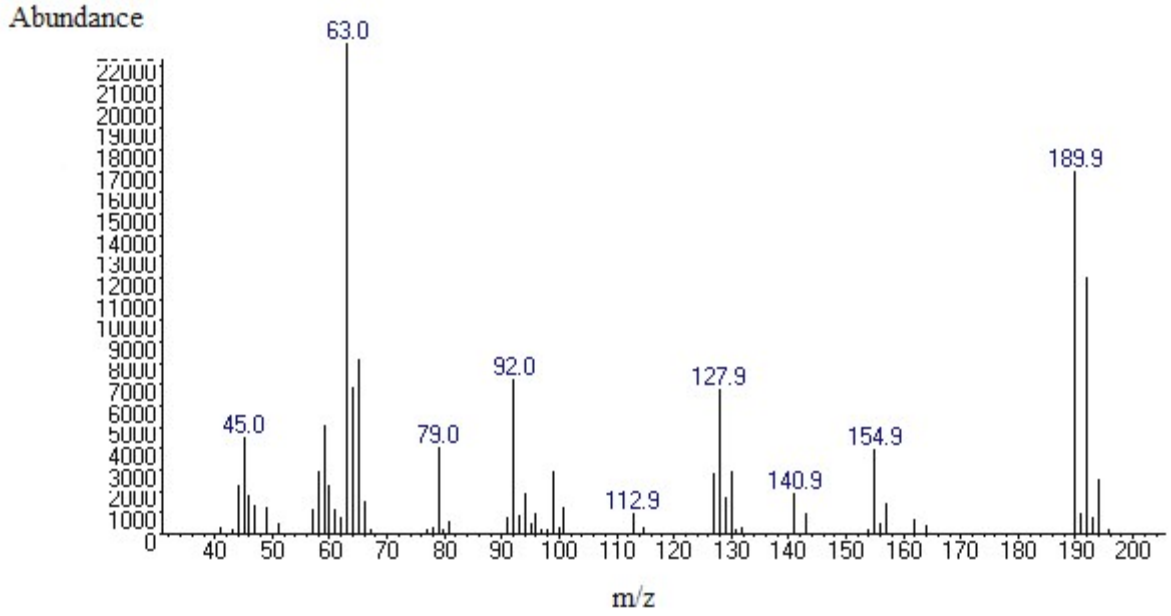


Figure-S6: Mass spectrum of SM disulfide

Name: Disulfide, bis(2-chloroethyl) (Bis(2-chloroethyl) disulfide)
Formula: $C_4H_8Cl_2S_2$
MW: 190 CAS#: 1002-41-1 NIST#: 273398 ID#: 6901 DB: replib
Other DBs: None
Contributor: A.A.Kutin, 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 |

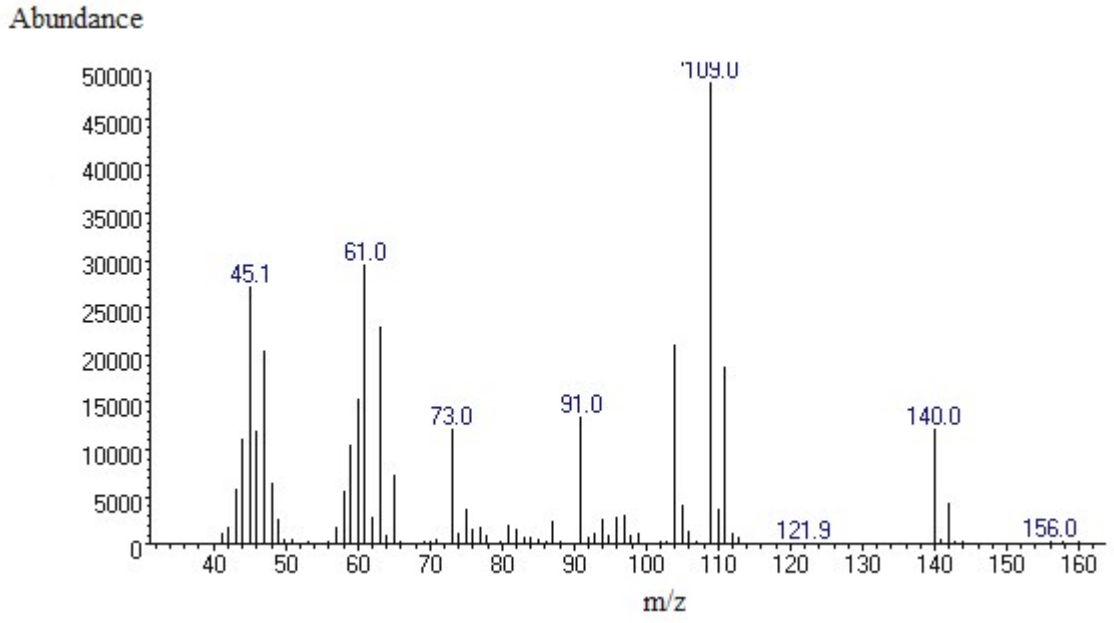


Figure-S7: Mass spectrum of Hemi sulphur mustard

Name: Ethanol, 2-(2-chloro-ethylthio)- (Hemisulfur mustard)
Formula: C_4H_9ClOS
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:

45 999 |	61 908 |	47 749 |	109 735 |	63 662 |
60 506 |	44 417 |	46 392 |	91 325 |	59 321 |

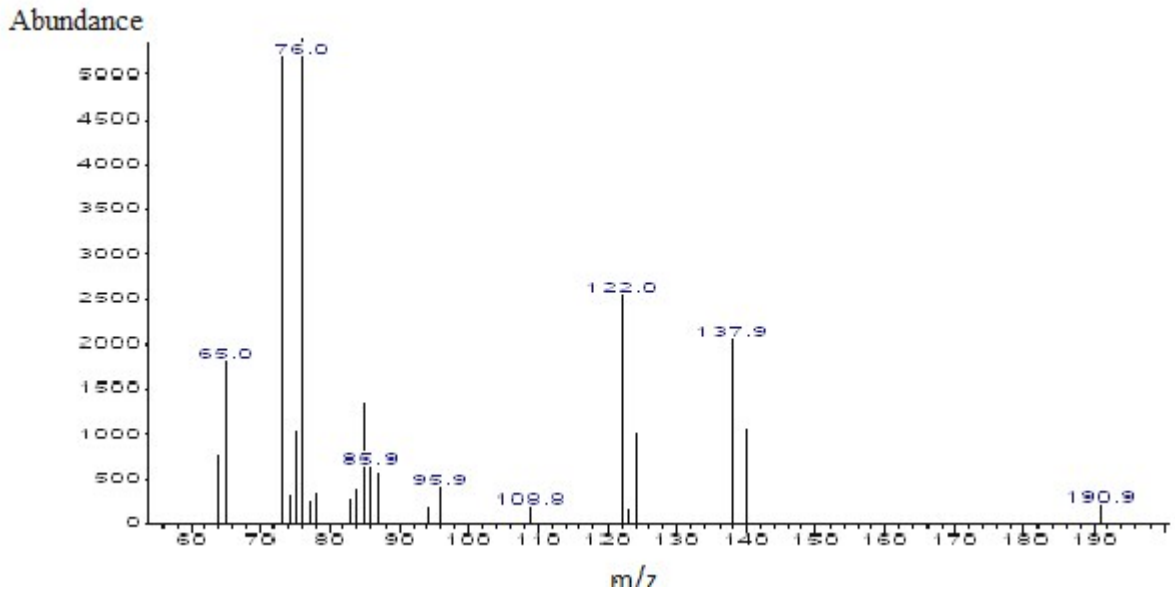


Figure-S8: Mass spectrum of chloro ethyl vinyl sulfoxide

Formula: C_4H_7ClOS (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:

76 999 |	63 881 |	138 369 |	65 241 |	58 193 |
59 193 |	75 146 |	140 142 |	47 132 |	73 115 |

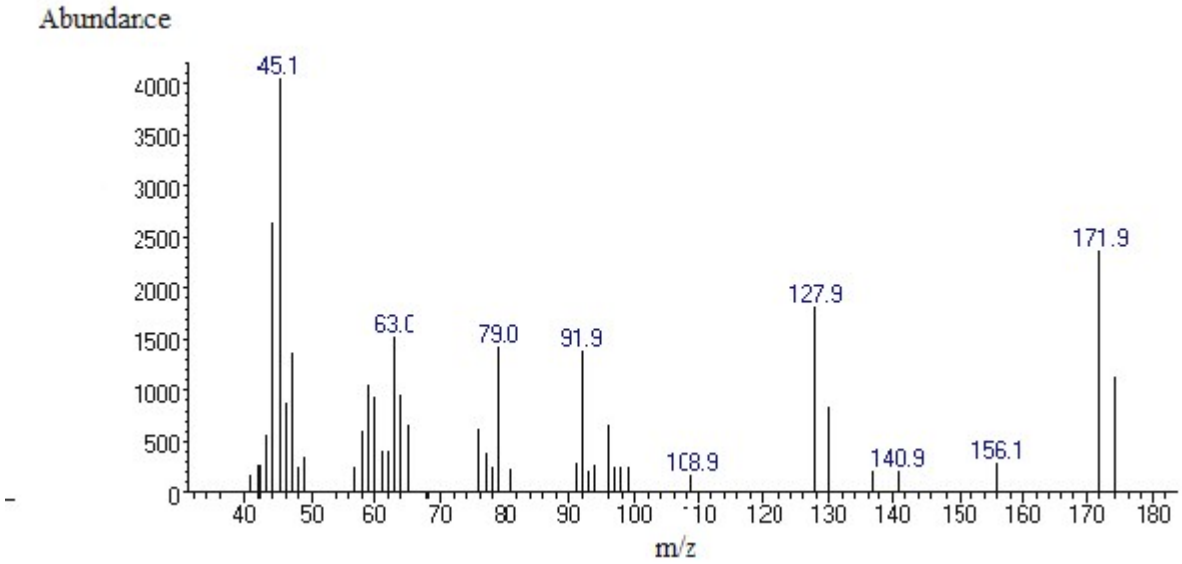


Figure-S9: Mass spectrum of 2-(2-Chloro-ethyldisulfanyl)-ethanol

Name: Ethanol, 2-[(2-chloroethyl)dithio]- (2-[(2-Chloroethyl)disulfanyl]ethanol)
Formula: $C_4H_9ClOS_2$
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 |

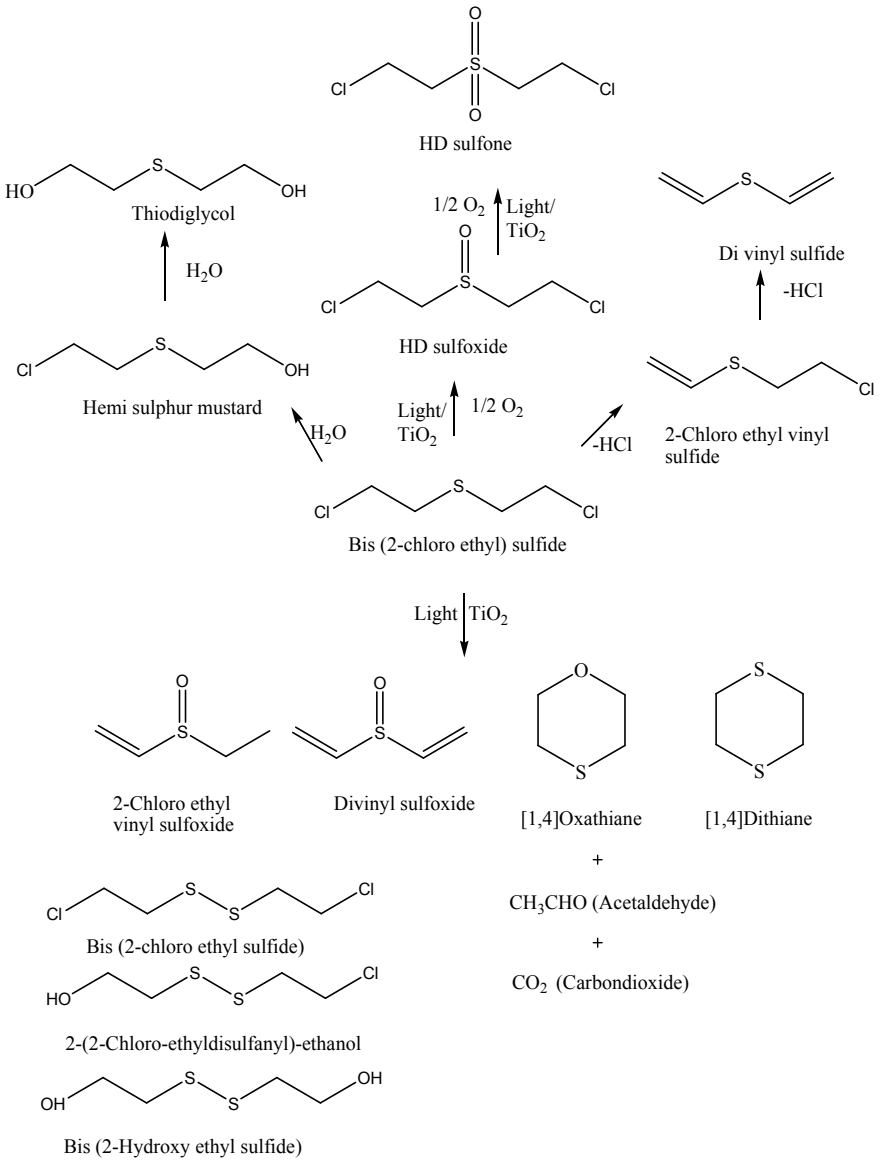


Figure-S10: Mechanism of photocatalytic degradation of sulphur mustard.

Table S1: Toxicity of degraded materials

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

LD_{50} = median lethal dose; LD_{LO} = lowest lethal dose; ip = intraperitoneal; iv = intravenous; sc = subcutaneous; NA-Not available

References

R1. N. B. Munro, S. S. Talmage, G. D. Griffin, L. C. Waters, A. P. Watson, J. F. King and V. Hauschild, *Environ. Heal. Persp.,* **1999**, 107, 933-974.

R2. D. M. Mizrahi, M. Goldvaser, I. Columbus, *Environ. Sci. Technol.,* **2011**, 45, 3466–3472.