

## Supplementary Data

### Degradation of sulfadiazine in water by UV/O<sub>3</sub> process: Performance and degradation pathway

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Table S1 Lengths of bonds in SDZ molecule

Bond	Values	Bond	Values	Bond	Values	Bond	Values
R(1, 2)	1.3914	R(4, 5)	1.3428	R(8, 11)	1.7671	R(14, 15)	1.4134
R(1, 6)	1.3395	R(5, 6)	1.337	R(11, 12)	1.4024	R(14, 17)	1.3724
R(1, 18)	1.0876	R(5, 7)	1.3918	R(11, 16)	1.4009	R(15, 16)	1.3859
R(2, 3)	1.3942	R(7, 8)	1.7032	R(12, 13)	1.385	R(15, 24)	1.0858
R(2, 19)	1.0827	R(7, 21)	1.0143	R(12, 22)	1.0845	R(16, 25)	1.0827
R(3, 4)	1.337	R(8, 9)	1.465	R(13, 14)	1.4143	R(17, 26)	1.0097
R(3, 20)	1.0877	R(8, 10)	1.4702	R(13, 23)	1.0858	R(17, 27)	1.0097

Table S2 Charges of atoms in SDZ molecule

Atoms	charges	Atoms	charges	Atoms	charges	Atoms	charges
1C	0.065	8S	2.332	15C	-0.294	22H	0.274
2C	-0.344	9O	-0.957	16C	-0.190	23H	0.262
3C	0.063	10O	-0.978	17N	-0.851	24H	0.262
4N	-0.525	11C	-0.402	18H	0.252	25H	0.279
5C	0.580	12C	-0.199	19H	0.275	26H	0.441
6N	-0.528	13C	-0.289	20H	0.253	27H	0.440
7N	-0.895	14C	0.194	21H	0.479		