

Supporting Information

The Initial Steps of Thermal Decomposition of TKX-50 (Dihydroxylammonium 5,5'-bistetrazole-1,1'-diolate) Crystals from Quantum Mechanics

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Table S1. The bond type and bond cut-off table in the fragment analysis.

Bond type	r _{cut-off} (Å)
C-C	2.31
C-H	1.63
C-O	2.15
C-N	2.20
H-H	1.11
H-O	1.50
H-N	1.61
O-O	2.22
O-N	2.10
N-N	2.17

Table S2. The electronic energy of species in Figure S2 calculated with different functionals at 6-311++G** basis set. B3LYP is the functional that best reproduces the CCSD(T) results, especially the STS2, the rate determining step.

	B3LYP	PBE	m06	m06-2x	CCSD(T)
STS1	25.8	23.1	26.4	32.5	28.4
SInt1	9.3	10.4	8.1	14.4	12.7
STS2	40.0	44.4	41.4	46.6	40.3
SProduct1	-44.0	-32.8	-43.7	-41.6	-45.4
STS3	47.2	45.2	48.7	55.4	48.6
SProduct2	17.5	23.5	18.4	24.4	17.9

Table S3. The electronic energy of species in Figure S3 calculated with different functionals in 6-311++G** basis set. B3LYP is the functional that best reproduces the CCSD(T) results, especially the STS5, the rate determining step.

	B3LYP	PBE	m06	m06-2x	CCSD(T)
STS4	22.6	19.3	24.5	30.6	26.0
SInt2	-0.4	0.5	-0.5	6.0	3.7
STS5	37.0	43.4	39.1	44.3	37.0
SProduct3	-40.0	-28.8	-38.4	-36.8	-42.4
STS6	43.6	42.3	46.1	52.4	43.9
SProduct4	21.5	28.3	22.8	28.2	19.9

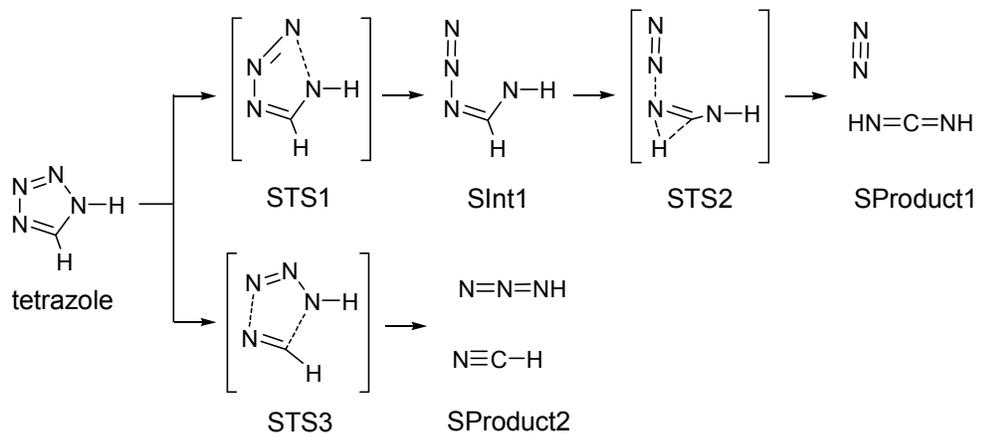


Figure S1. The decomposition mechanism of tetrazole.

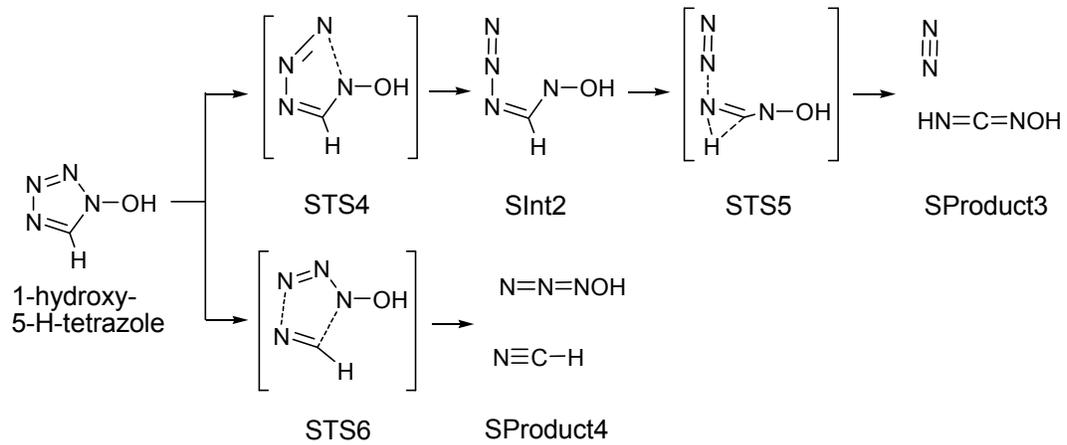


Figure S2. The decomposition mechanism of 1-hydroxy-5-H-tetrazole

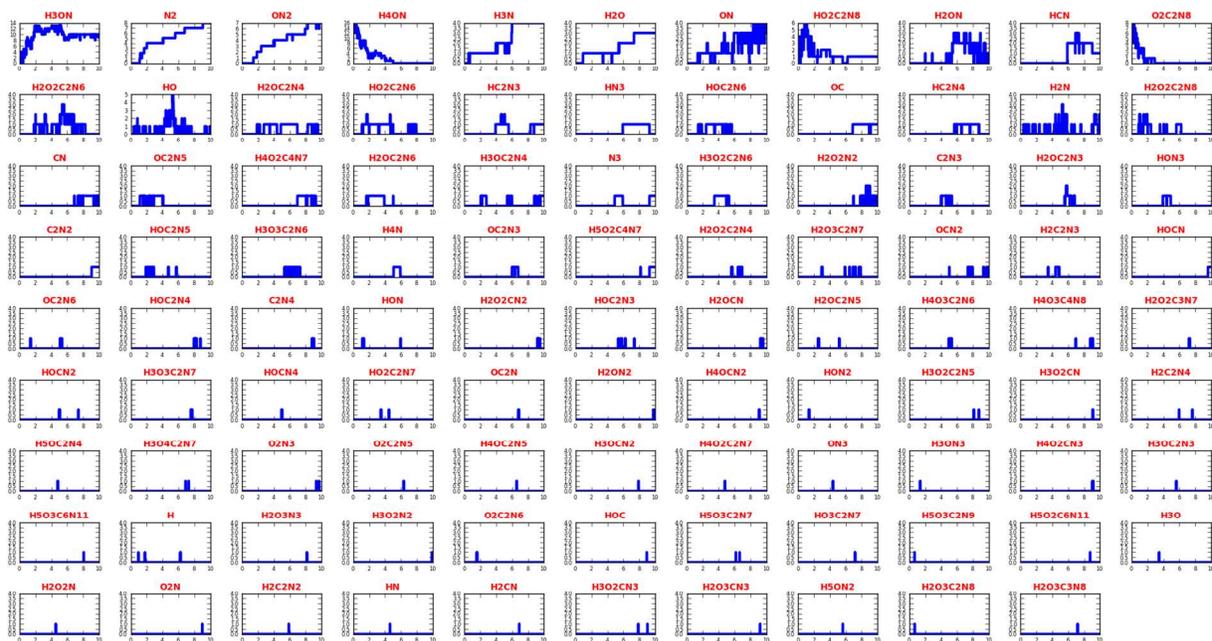


Figure S3. The fragments distribution as a function of time (12 ps) at 1750 K. Every single sub-figure stands for one fragment. Here, we show all the fragments observed in the simulation.