Supplementary Information for

Gas-Phase Formation of Silicon Monoxide via Non-Adiabatic Reaction Dynamics and its Role as a Building Block of Interstellar Silicates

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Table S1. Peak velocities (V_p) and speed ratios (S) of the silicon (Si), and oxygen (O_2) beams along with the corresponding collision energies (E_C) and center-of-mass angles (Θ_{CM}).

Beam	V_p (m s^{-1})	S	E_C (kJ mol^{-1})	Θ_{CM} (degree)
Si (^3P)	952 ± 15	6.1 ± 0.6		
$^{18}O_2$ ($X^3\Sigma_g^-$)	760 ± 20	13.8 ± 1.0	11.7 ± 0.5	46.5 ± 1.2

Table S2. The root-mean-square deviation (RMSD) of each TOF of single channel and two-channel fit.

	Single channel fit	Two-channel fit
22.25°	6.43	6.05
28.25°	5.11	4.38
34.25°	2.95	2.83
40.25°	2.16	2.25
46.25°	3.31	3.51
52.25°	2.61	2.77

Table S3. The relative energies (in kJ mol^{-1}) of products, intermediates, and transition states with respect to the separated reactants (Si (^{3}P) + O_2 ($X^3\Sigma_g^-$)).

	Experimental[1]	CCSD(T)/CBS[2]	CASSCF/Def2-TZVP[3]	MRCI/Def2-TZVP[c]
SiO($X^1\Sigma^+$) + O(^{3}P)	-301	-301	-384	-303
SiO($X^1\Sigma^+$) + O(^{1}D)	-112	-90	-174	-107
i1			-473	-420
i2			-160	-99
i3			-407	-410
i4			-648	-650
i5			-255	-183
TSr2			39	66
TS14			-366	-352
TS15			-226	-132
TS2p			-153	-93
TS3p			-332	-271

Note:
Experimental heat of reaction is computed from the heat of formation [1-3].
[2] Geometries and ZPEs are calculated at CCSD(T)/cc-pVTZ level. CBS are extrapolated from 3-, 4-, and 5-zeta basis sets.
[3] Geometries and ZPE are calculated at CASSCF/Def2-TZVP level.

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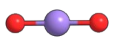
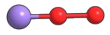
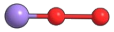
Table S4. The relative energies (in kJ mol^{-1}) of the lowest singlet and triplet electronic state of intermediates and transition states with respect to the separated reactants (Si (^3P) + O_2 ($X^3\Sigma_g^-$). The first column indicates whether the species is optimized on the singlet (S) or triplet (T) surface.

	Optimal Structure on Surface	Singlet Energy	Triplet Energy
i1	S	-425	-179
i2	T	-151	-101
i3	T	-464	-415
i4	S	-660	-161
i5	S	-186	32
TSr2	T	51	66
TS14	S	-351	-384
TS15	S	-133	-86
TS2p	T	-131	-90
TS3p	T	-247	-270

Table S5. The point group, electronic state, and geometric parameters of each stationary point.

Structure								
Name	i1	i3	i4	TS14	TS3p	MSX-a1	MSX-a2	MSX-c
Point Group	C_{2v}	C_{2v}	$D_{\infty h}$	C_{2v}	C_s	C_{2v}	C_{2v}	C_s
Electronic State	$^1A_1$	$^3B_2$	$_1\Sigma_g^+$	$^1A_1$	^3A”	-	-	-
O-Si-O Bond Angle (°)	58.42	110.83	180.00	96.81	119.56	86.71	104.68	114.4
Si-O Bond Length (pm)	166.4	159.7	151.4	166.6	152.6	166.1	161.4	152.8
Si-O Bond Length (pm)	166.4	159.7	151.4	166.6	214.6	166.1	161.4	203.2
Structure								
Name	i2	i5	TSr2	TS15	TS2p	SiO	O_2	MSX-b
Point Group	C_s	$C_{\infty v}$	C_s	C_s	C_s	$C_{\infty v}$	$D_{\infty h}$	$C_{\infty v}$
Electronic State	^3A”	$_1\Sigma^+$	^3A”	^1A’	^3A”	$^1A_1$	$_3\Sigma_g^-$	-
Si-O-O Bond Angle (°)	110.40	180.00	118.68	121.41	109.98	-	-	180.00
Si-O Bond Length (pm)	170.9	151.8	253.5	153.0	164.7	152.2	-	151.7
O-O Bond Length (pm)	141.1	144.2	124.0	159.9	157.7	-	121.7	170.7

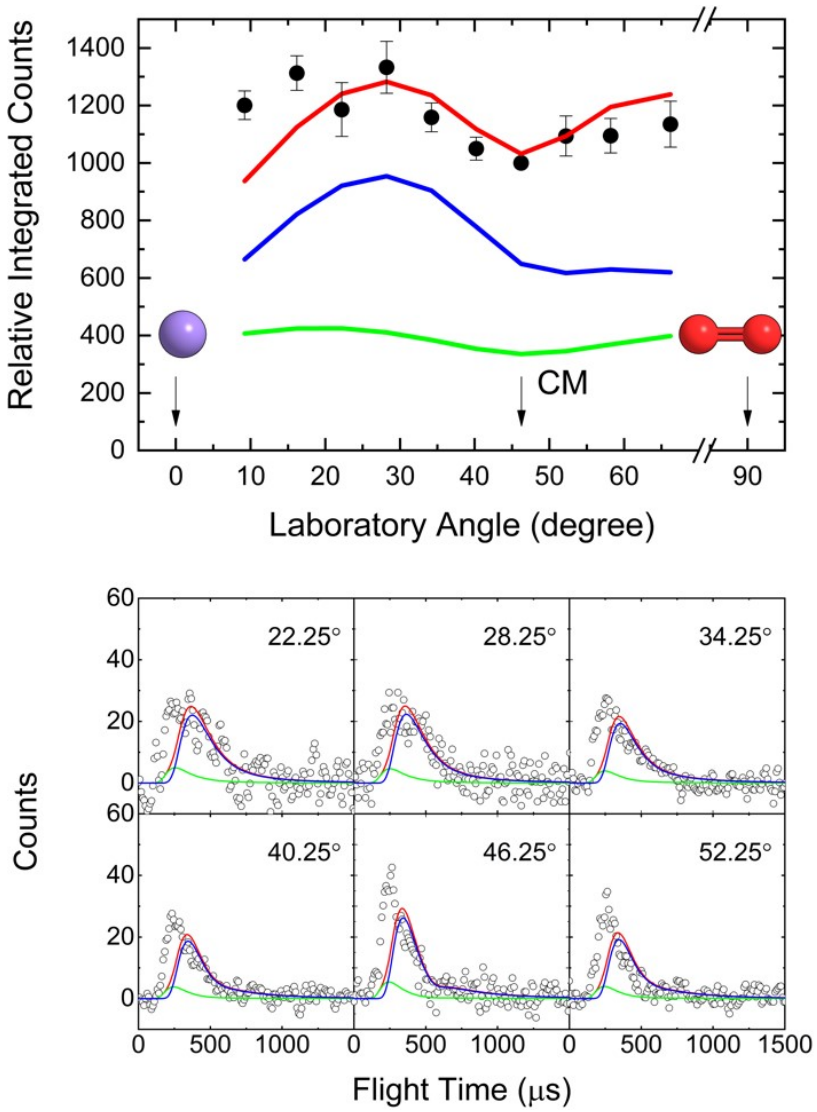


Figure S1. Laboratory angular distribution (top) and time-of-flight (TOF) spectra (bottom) recorded at m/z = 46 for the reaction of the silicon atom (Si; ^{3}P) with molecular oxygen ($^{18}O_2$; $X^3\Sigma_g^-$). The data were fit with two channels: i) ^{28}Si (^{3}P; 28 amu) + $^{18}O_2$ ($X^3\Sigma_g^-$; 36 amu) → $^{28}Si^{18}O$ ($X^1\Sigma^+$; 46 amu) + ^{18}O (^{3}P; 18 amu) (green), ii) ^{28}Si (^{3}P; 28 amu) + $^{18}O_2$ ($X^3\Sigma_g^-$; 36 amu) → $^{28}Si^{18}O$ ($X^1\Sigma^+$; 46 amu) + ^{18}O (^{1}D; 18 amu) (blue), with branching ratios of 33% (channel i) and 67% (channel ii), respectively. CM represents the center-of-mass angle, and 0° and 90° define the directions of the silicon atom and molecular oxygen beams, respectively. The black circles depict the experimental data, and colored lines the fits (red corresponding to the total fit).

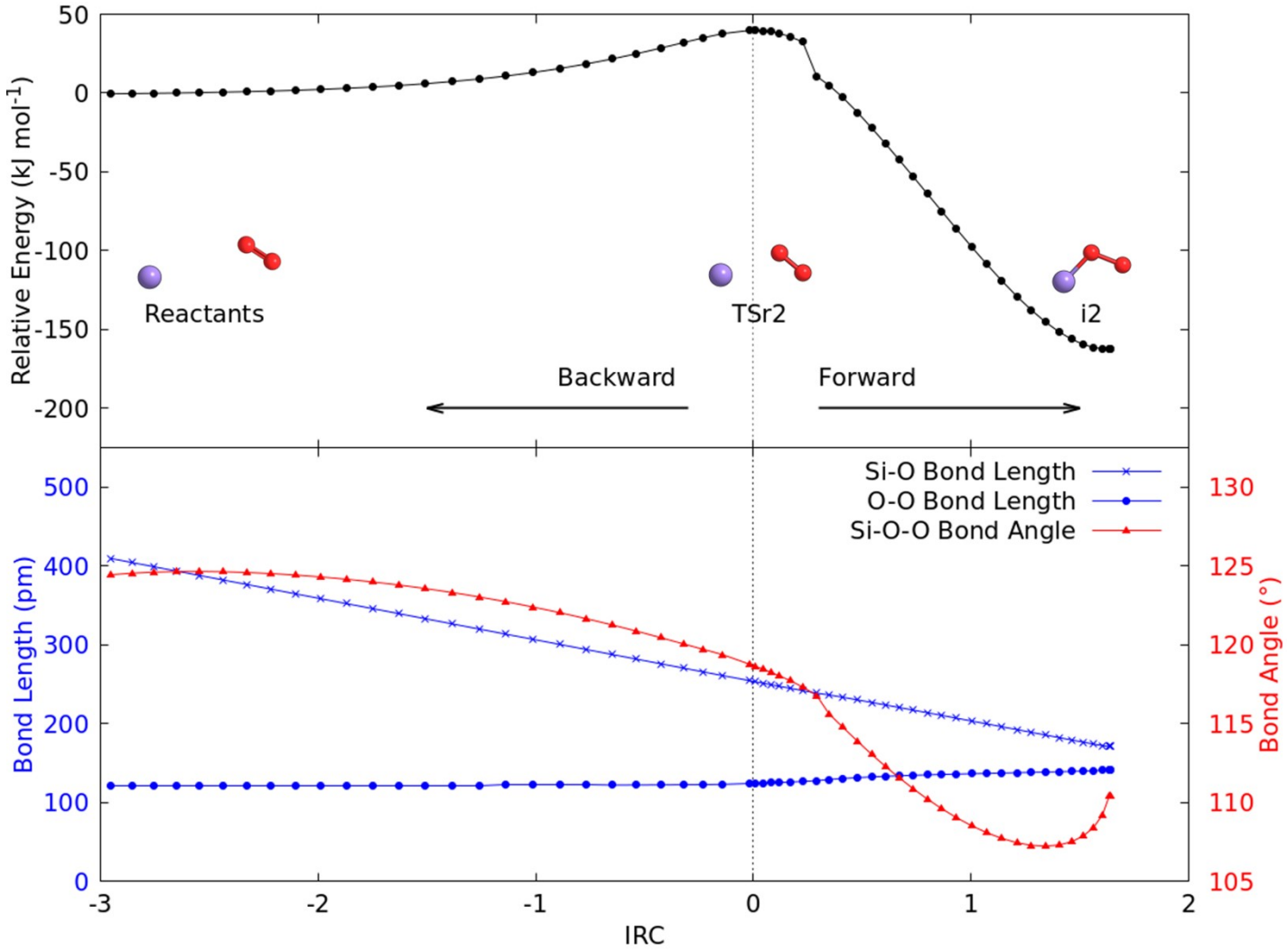


Figure S2. The intrinsic reaction coordinate (IRC) demonstrating that **TSr2** connects to the separated reactants and **i2**. The energies is in kJ mol^{-1} calculated with CASSCF/def2-TZVP (upper figure) and the geometrical parameters are pm and degree (lower figure).

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