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Supplement of

**MP CBM-Z V1.0: design for a new Carbon Bond Mechanism Z (CBM-Z)
gas-phase chemical mechanism architecture for next-generation proces-
sors**

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Table S1. Initial concentrations used in the one-point test case.

Species	Initial Value(ppb)	Species	Initial Value(ppb)
H ₂ SO ₄	0.5	TOL	6.7
HNO ₃	3.4	XYL	2.8
HCL	9.8E-21	CRES	6.7E-02
NH ₃	2.1	TO ₂	1.8E-03
NO	1.5	CRO	8.9E-06
NO ₂	19.0	OPEN	0.8
NO ₃	1.4E-03	ONIT	11.7
N ₂ O ₅	8.7E-03	ROOH	0.4
HONO	0.2	RO ₂	7.0E-04
HNO ₄	0.1	ANO2	1.4E-04
O ₃	89.4	NAP	1.7E-03
O(¹ D)	1.3E-12	XO ₂	1.2E-02
O(³ P)	1.6E-06	XPAR	5.1E-04
OH	3.4E-04	ISOP	9.0E-02
HO ₂	3.2E-02	ISOPRD	0.6
H ₂ O ₂	4.9	ISOPP	4.8E-04
CO	1930.3	ISOPN	1.3E-05
SO ₂	0.9	ISOPO ₂	4.9E-04
CH ₄	1761.4	DMS	9.8E-21
C ₂ H ₆	1.6E-02	MSA	9.8E-21
CH ₃ O ₂	4.0E-03	DMSO	9.8E-21
ETHP	5.5E-05	DMSO ₂	9.8E-21
HCHO	11.0	CH ₃ SO ₂ H	9.8E-21
CH ₃ OH	1.0	CH ₃ SCH ₂ OO	9.8E-21
ANOL	1.5E-21	CH ₃ SO ₂	9.8E-21
CH ₃ OOH	0.5	CH ₃ SO ₃	9.8E-21
ETHOOH	5.8E-02	CH ₃ SO ₂ OO	9.8E-21
ALD2	5.1	CH ₃ SO ₂ CH ₂ OO	9.8E-21
HCOOH	4.7	SULFHOX	9.8E-21
RCOOH	4.3	TERP	9.8E-21
C ₂ O ₃	1.5E-03	SOA1	9.8E-21
PAN	5.9	SOA2	9.8E-21
PAR	12.3	SOA3	9.8E-21
AONE	9.7	SOA4	9.8E-21
MGLY	1.0	SOA5	9.8E-21
ETH	2.9	SOA6	9.8E-21
OLET	3.6	ASO ₄	9.8E-21
OLEI	6.5E-02	ANO ₃	9.8E-21

Pressure = 1.0 atm; Relative humidity = 58%; Temperature = 304K.

