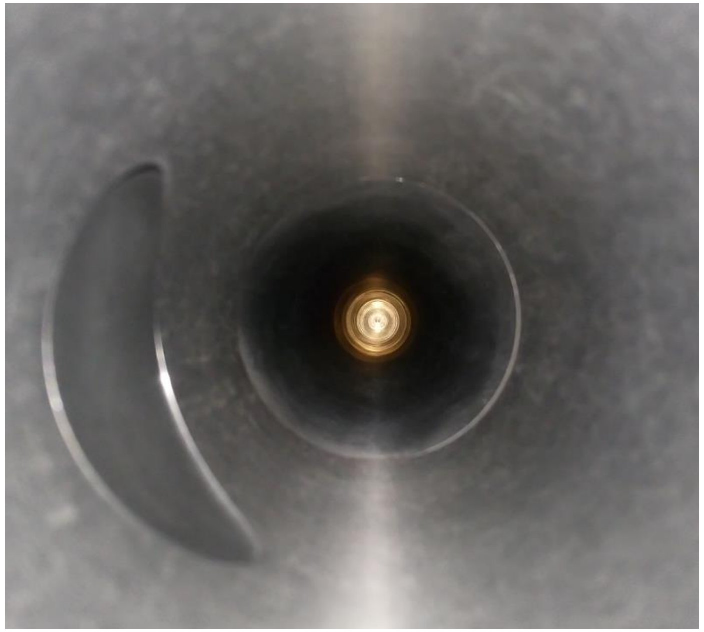
INTRACAVITY LASER ABSORPTION SPECTROSCOPY DIAGNOSTICS OF GAS-PHASE FEO ABSORPTION CROSS SECTION IN A SHOCK TUBE



The 33rd Annual Symposium of the Isreali Section of the Combustion Institute

M.R. LALANNE OPEN UNIVERSITY OF ISRAEL

FLAME MADE MATERIAL

>$ 15 Billions/ yr

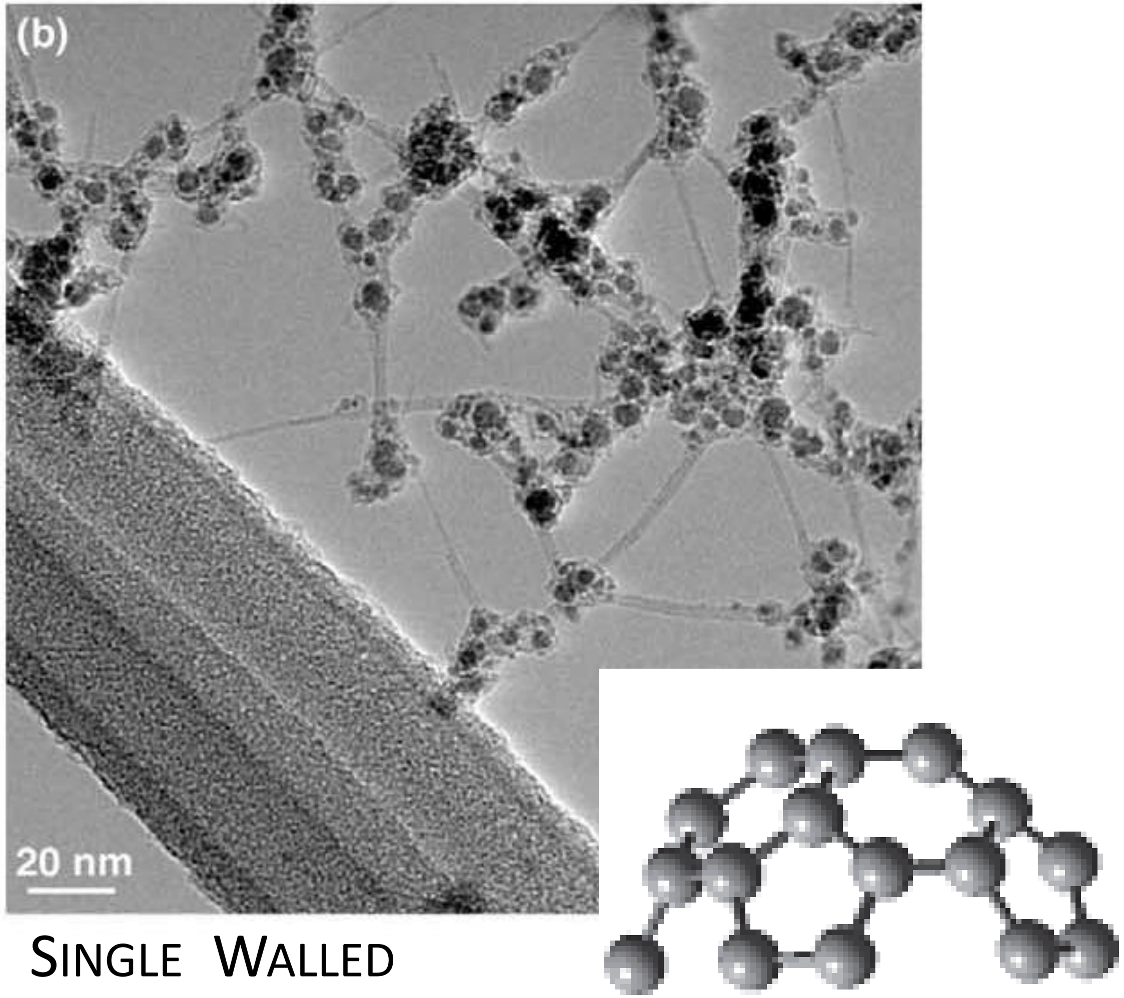
Li-doped $Na_2O.xA_{l2}O_3$
Li-ZnO
$LiMnO_4$
Borosilicate glass
$BaCO_3$
C-Co
C-Cu
Pt/C C/Pt
$CaCO_3$
Bioglass
CaF_2, SrF_2,BaF_2
F-TiO_2, F-ZrO_2
NaCl
Mg-$Ca_3(PO_4)_2$
Ni:MgO-SiO_2
Mg_2SiO_4:Cr
MgO
MgO-Al_2O_3
MgO-Fe_2O_3
MgO-Al_2O_3
3Al_2O_3.2SiO_2

Al_2O_3: Ce
$CoO_{x-}Al_2O_3$
NiO-Al_2O_3
ZrO_2-Al_2O_3
Al_2O_3
MgO-Al_2O_3
$Y_3Al_5O_{12}$
TiO_2/Al_2O_3
Al_2O_3/ZrO_2
$Al_2O_3/Ce_xZr_{1-x}O_2$
Hastelloy
Al_2O_3
Pt-Ba/Al_2O_3
Pd/La_2O_3/Al_2O_3
PT-Rh-Ru/Al_2O_3
Si coated Al-TiO_2
Pt-Pd/Al_2O_3

$Y_3Al_5O_{12}$
Alpha Al_2O_3
SiO_2, SiO_2/ZnO
Ni:MgO-SiO_2
SiO_2, SiO_2/ZnO_2
Yb_2O_3/SiO_2
Ta_2O_5/SiO_2
SiO_2/FeO_3
Ag/$Ca_3(PO_4)_2$
$FePO_4$
$CaSO_4$
Si-O_2-V_2O_5-WO_3-TiO_2
Au/TiO_2, Ag/TiO_2
$BiVO_4$
Mg_2SiO_4:Cr
Cr-WO_3
$LiMn_2O_4$
Mn_2O_3
$FePO_4$
Fe_2O_3
Fe-TiO_2
Au-Ag Fe_2O_3…::……………………

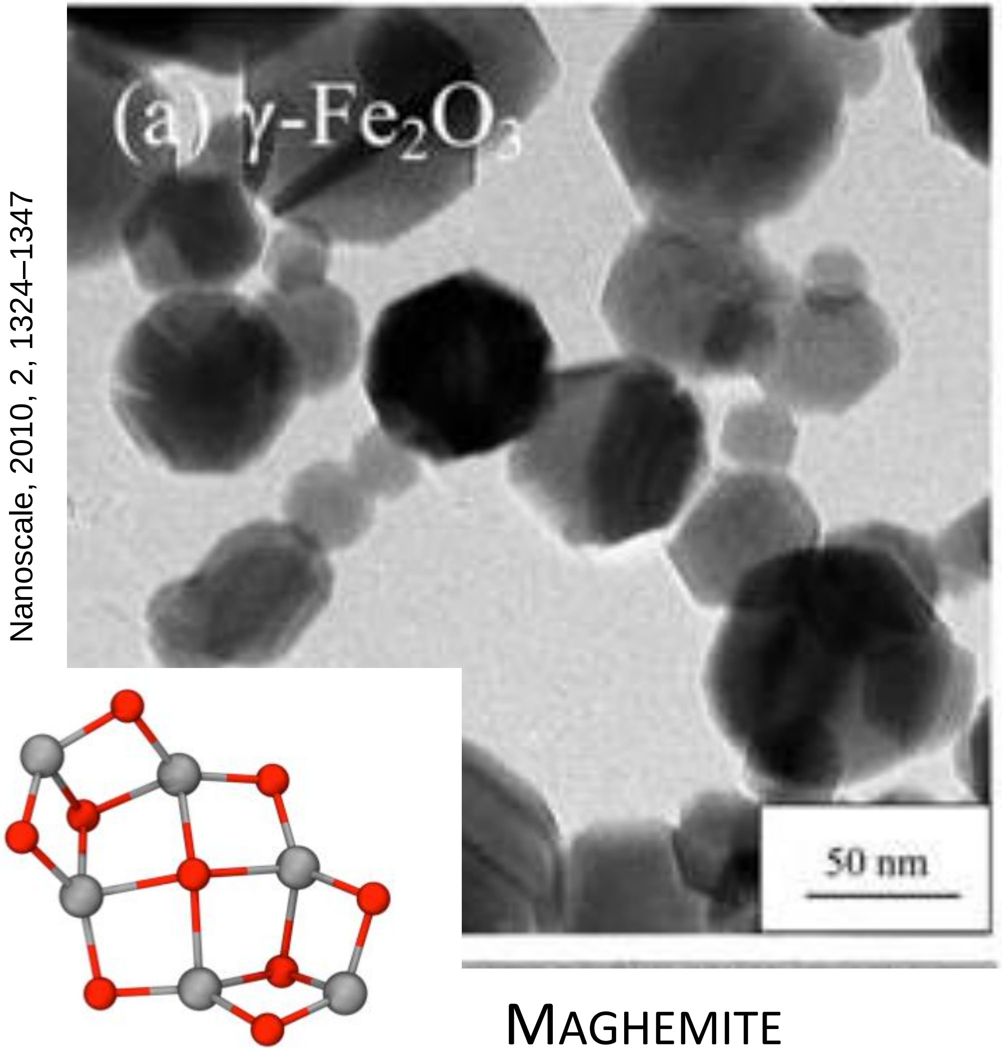
FLAME MADE MATERIAL

RANDALL L. VANDER WAL* and LEE J. HALL*COMBUSTION AND FLAME* 130:27–36 (2002



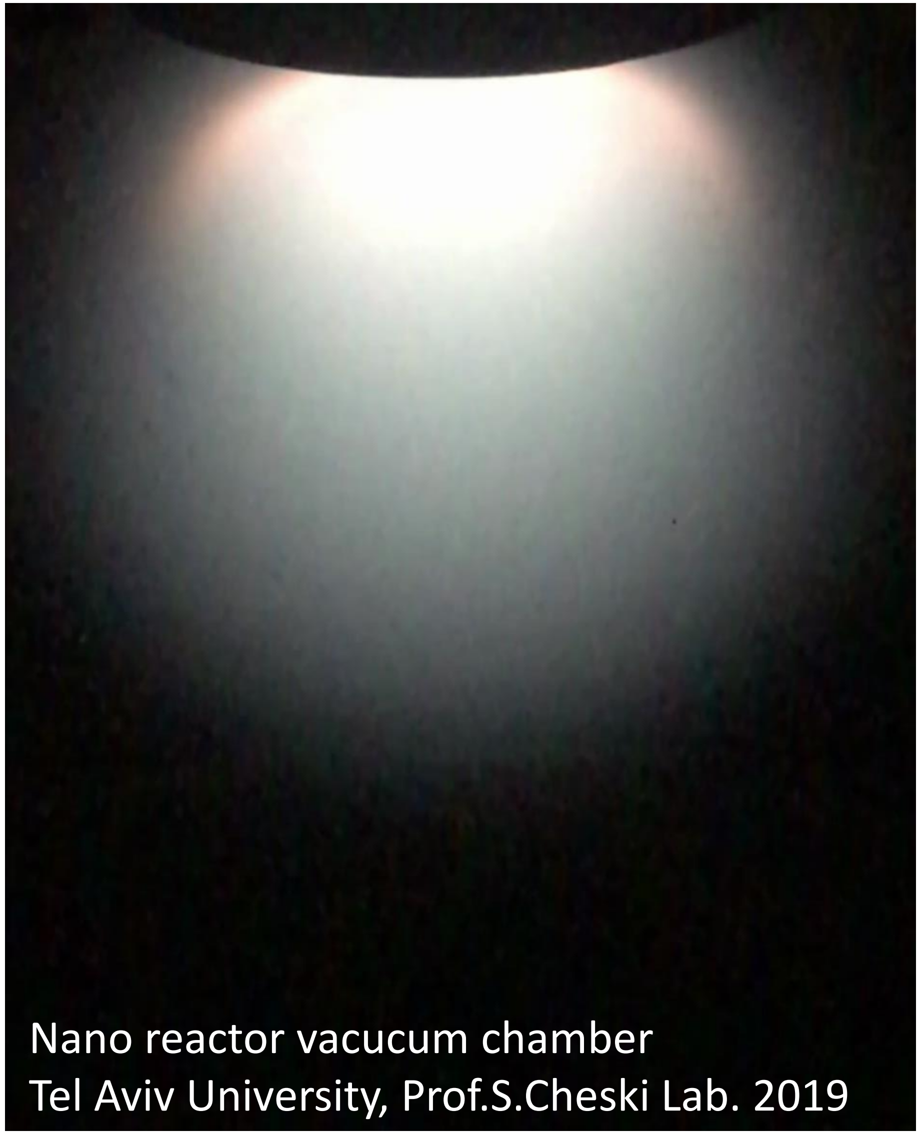
SINGLE WALLED CARBON NANOTUBES

Wey Yang Teoh,a Rose Amala and Lutz M€adler*b
Nanoscale, 2010, 2, 1324–1347



MAGHEMITE

IRON PENTACARBONYL DOTTED FLAME



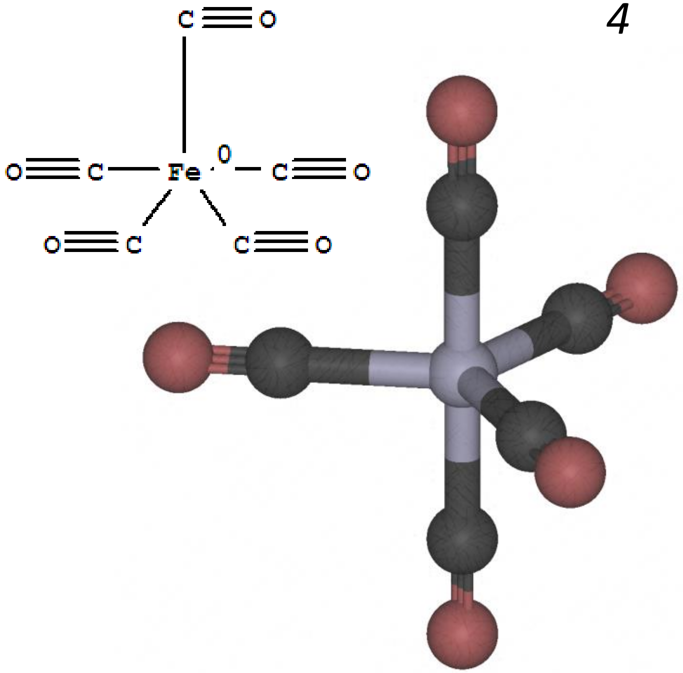
Nano reactor vacucum chamber
Tel Aviv University, Prof.S.Cheski Lab. 2019

IPC inhibitor
reducing burning velocities
Methane/air flame
Bonne et al. 1962

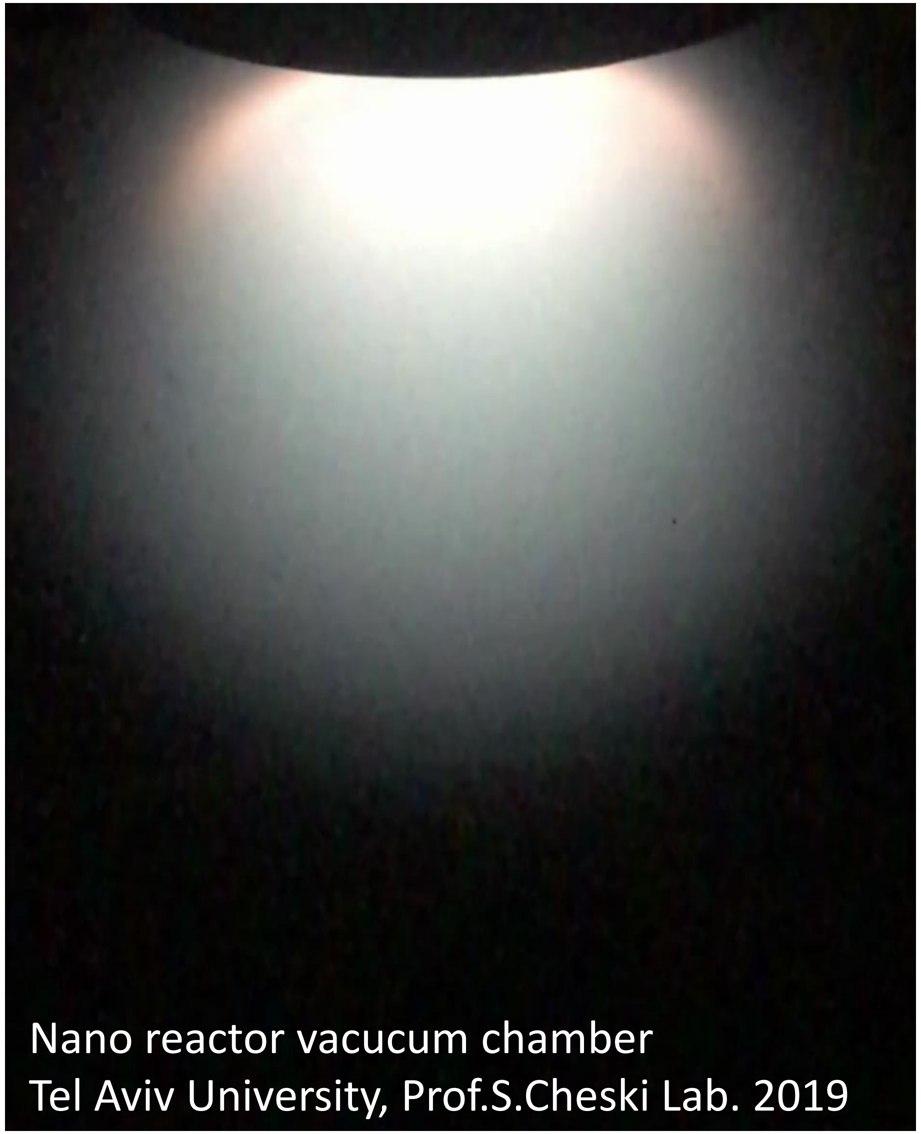
Low inhibition under 10^{-2} atm
Methane /oxygen flame
Milner et al. 1969

Inhibition decrease over 200 ppm
Oxygen/hydrogen flame low pressure
Linteris et al. 1996

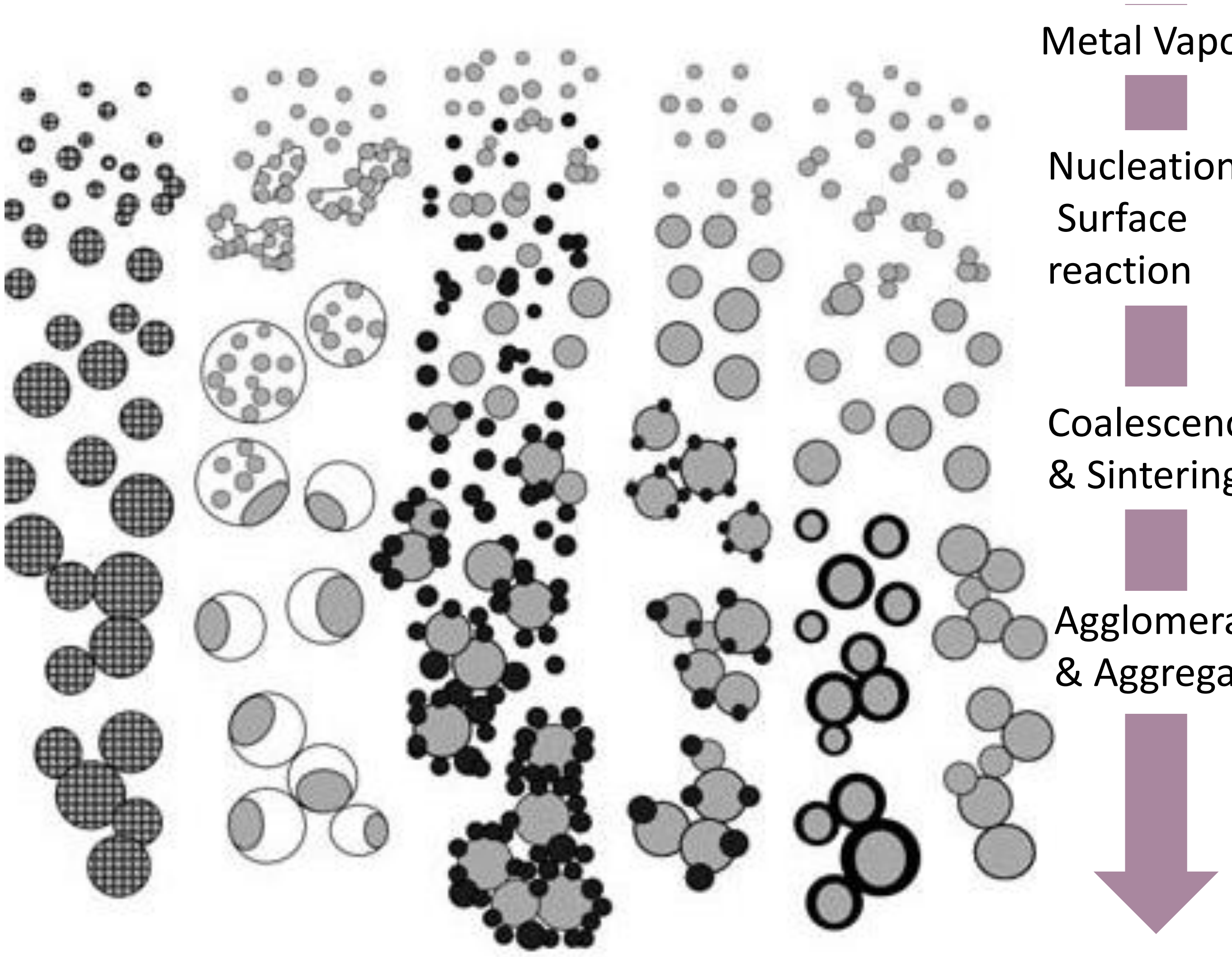
Inhibition or promotion
Air/hydrogen flame atm pressure
Babushock et al., 2009



Iron Pentacarbonyl Dotted Flame



Nano reactor vacucum chamber
Tel Aviv University, Prof.S.Cheski Lab. 2019



Metal Vapor

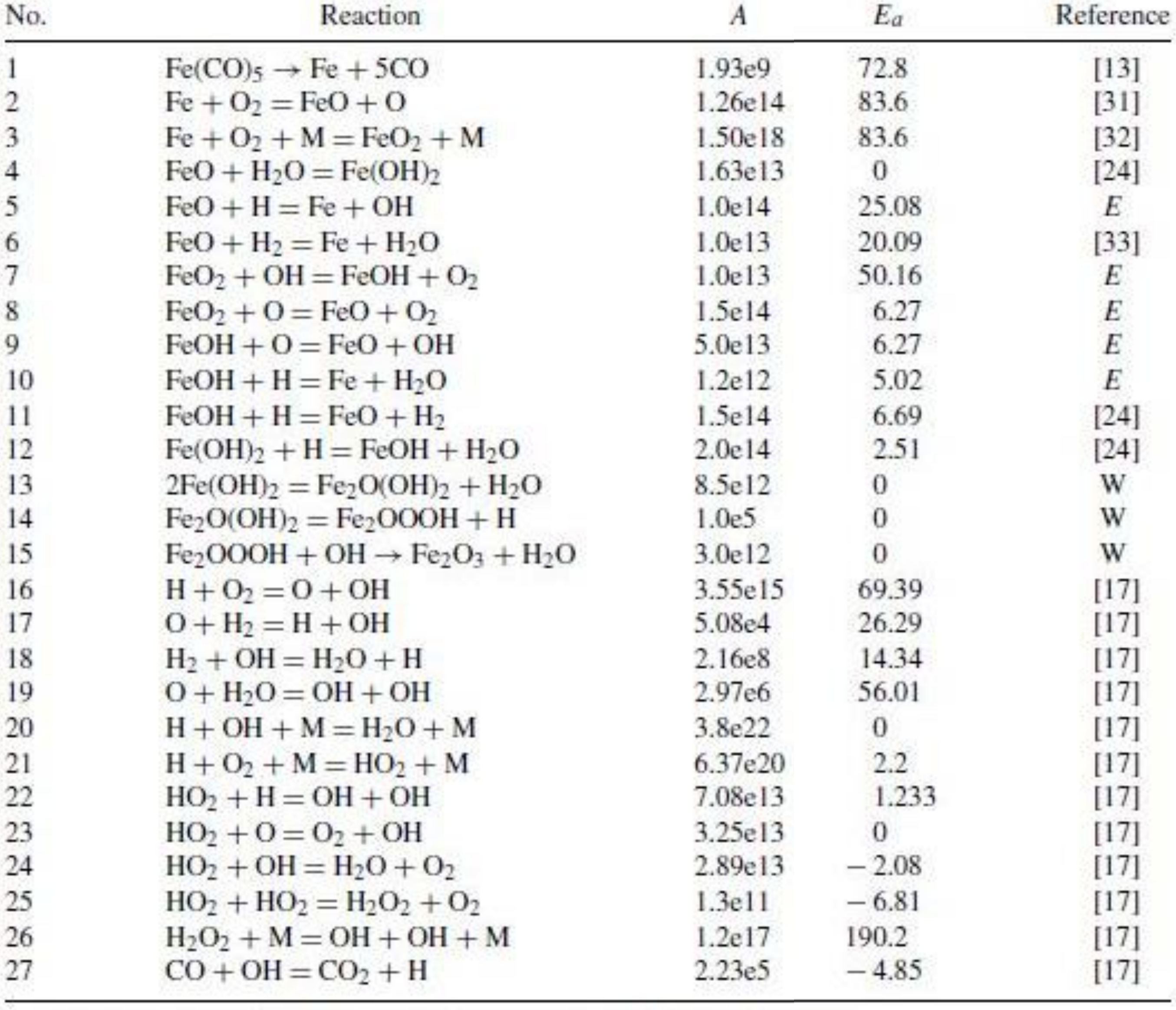
Nucleation & Surface reaction

Coalescence & Sintering

Agglomeration & Aggregation

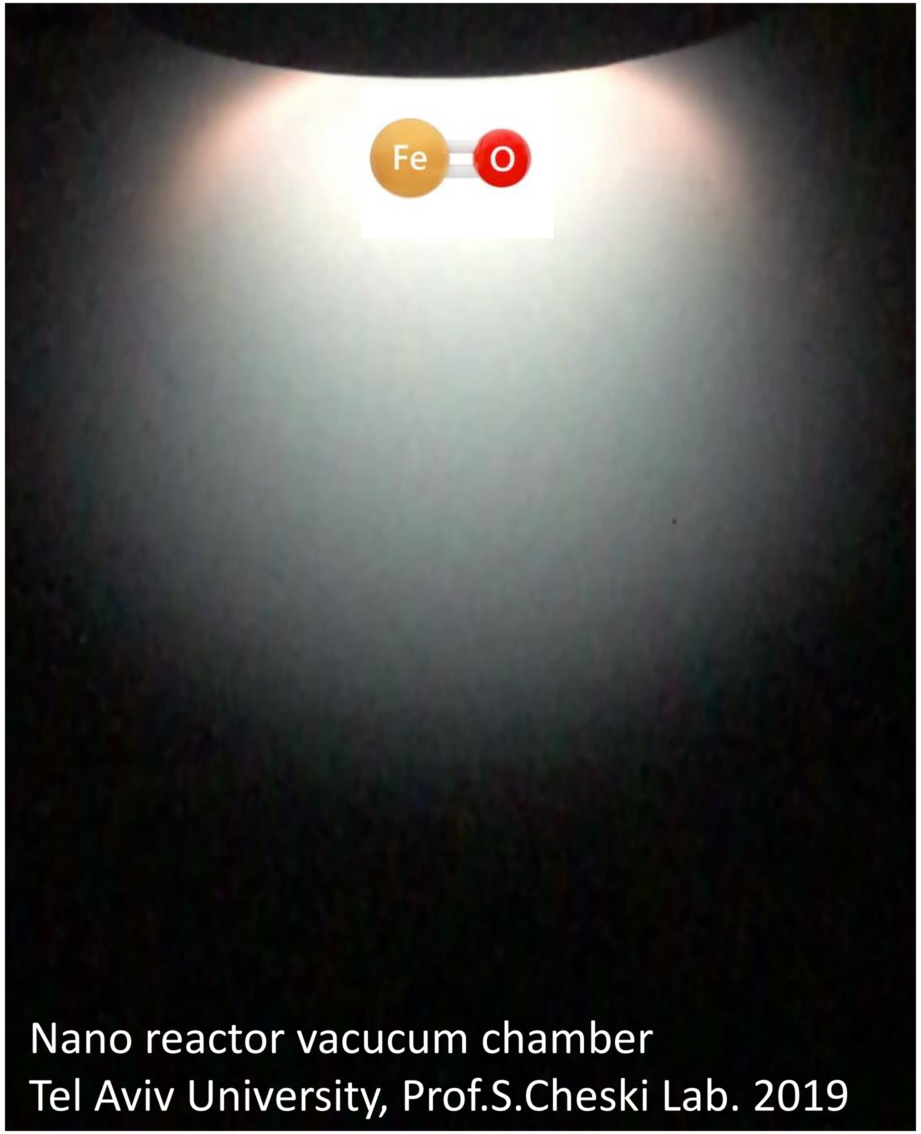
IRON PENTACARBONYL DOTTED FLAME

Nano reactor vacucum chamber
Tel Aviv University, Prof.S.Cheski Lab. 2019

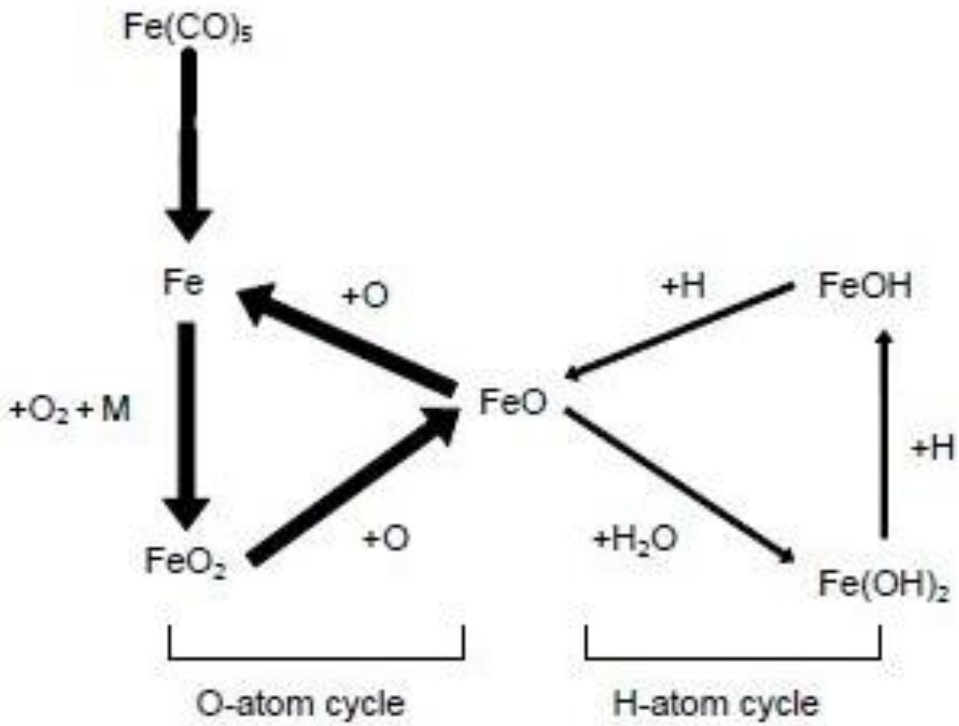


No.	Reaction	A	E_a	Reference
1	$Fe(CO)_5 \rightarrow Fe + 5CO$	1.93e9	72.8	[13]
2	$Fe + O_2 = FeO + O$	1.26e14	83.6	[31]
3	$Fe + O_2 + M = FeO_2 + M$	1.50e18	83.6	[32]
4	$FeO + H_2O = Fe(OH)_2$	1.63e13	0	[24]
5	$FeO + H = Fe + OH$	1.0e14	25.08	*E*
6	$FeO + H_2 = Fe + H_2O$	1.0e13	20.09	[33]
7	$FeO_2 + OH = FeOH + O_2$	1.0e13	50.16	*E*
8	$FeO_2 + O = FeO + O_2$	1.5e14	6.27	*E*
9	$FeOH + O = FeO + OH$	5.0e13	6.27	*E*
10	$FeOH + H = Fe + H_2O$	1.2e12	5.02	*E*
11	$FeOH + H = FeO + H_2$	1.5e14	6.69	[24]
12	$Fe(OH)_2 + H = FeOH + H_2O$	2.0e14	2.51	[24]
13	$2Fe(OH)_2 = Fe_2O(OH)_2 + H_2O$	8.5e12	0	W
14	$Fe_2O(OH)_2 = Fe_2OOOH + H$	1.0e5	0	W
15	$Fe_2OOOH + OH \rightarrow Fe_2O_3 + H_2O$	3.0e12	0	W
16	$H + O_2 = O + OH$	3.55e15	69.39	[17]
17	$O + H_2 = H + OH$	5.08e4	26.29	[17]
18	$H_2 + OH = H_2O + H$	2.16e8	14.34	[17]
19	$O + H_2O = OH + OH$	2.97e6	56.01	[17]
20	$H + OH + M = H_2O + M$	3.8e22	0	[17]
21	$H + O_2 + M = HO_2 + M$	6.37e20	2.2	[17]
22	$HO_2 + H = OH + OH$	7.08e13	1.233	[17]
23	$HO_2 + O = O_2 + OH$	3.25e13	0	[17]
24	$HO_2 + OH = H_2O + O_2$	2.89e13	-2.08	[17]
25	$HO_2 + HO_2 = H_2O_2 + O_2$	1.3e11	-6.81	[17]
26	$H_2O_2 + M = OH + OH + M$	1.2e17	190.2	[17]
27	$CO + OH = CO_2 + H$	2.23e5	-4.85	[17]

IRON OXYDE IN IRON DOTTED FLAME



Nano reactor vacucum chamber
Tel Aviv University, Prof.S.Cheski Lab. 2019



Radical recombination cycles,
Linteris et al. 2000

IRON OXYDE

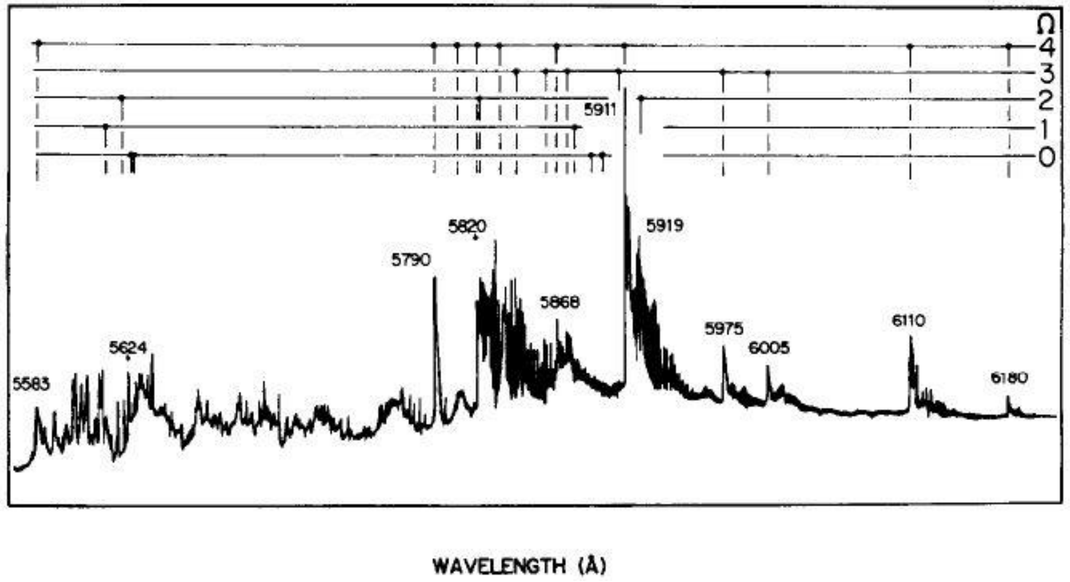
Orange syteme
(580 to 614 and 558 to 554 nm)
Delsemme.al, 1945

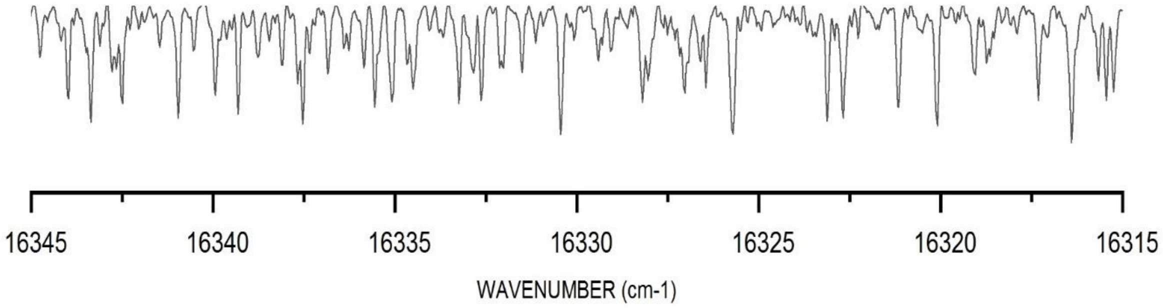
Ro-vibrational bands system studed
Cheung et al., 1983

Upper estimation of Abs. cross section
H.S Son et al 2000

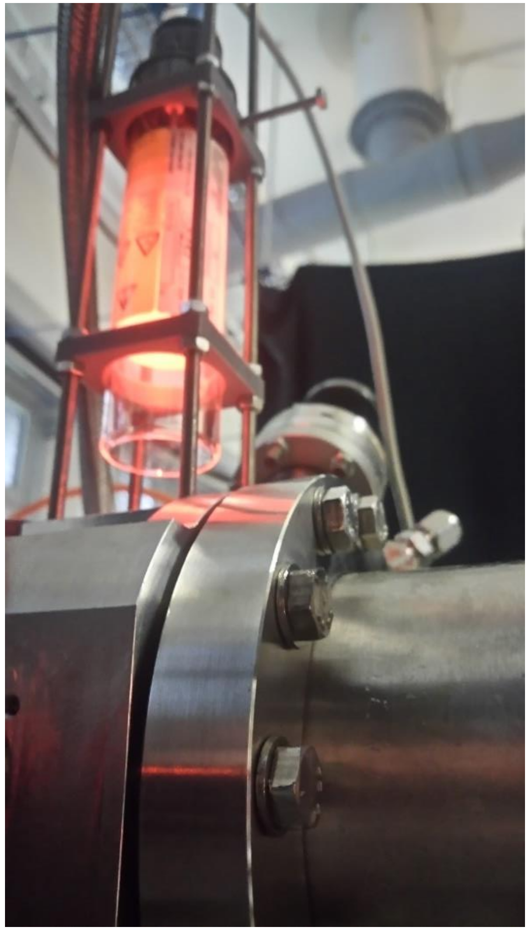
FeO/Fe equilibrium in Shock tube
Giesen et al. 2002

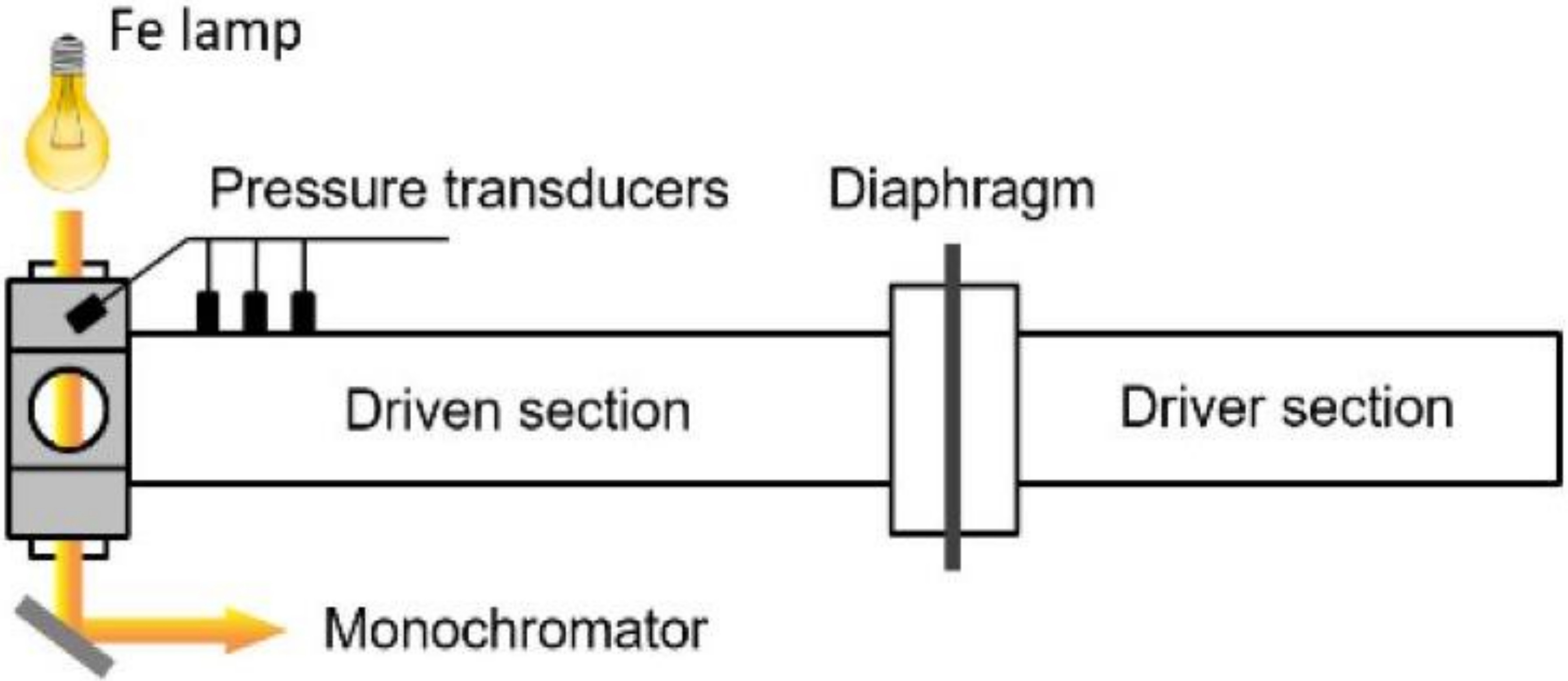
FeO detected in Flames
Rahinov et al. 2014





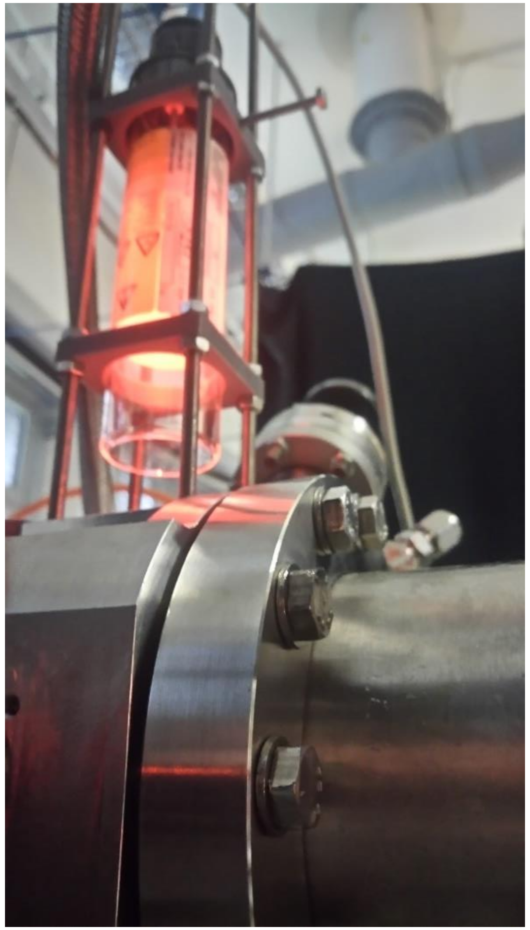
SHOCK TUBE & ATOMIC RESONANCE ABS.SPECTROSCPY (ARAS)

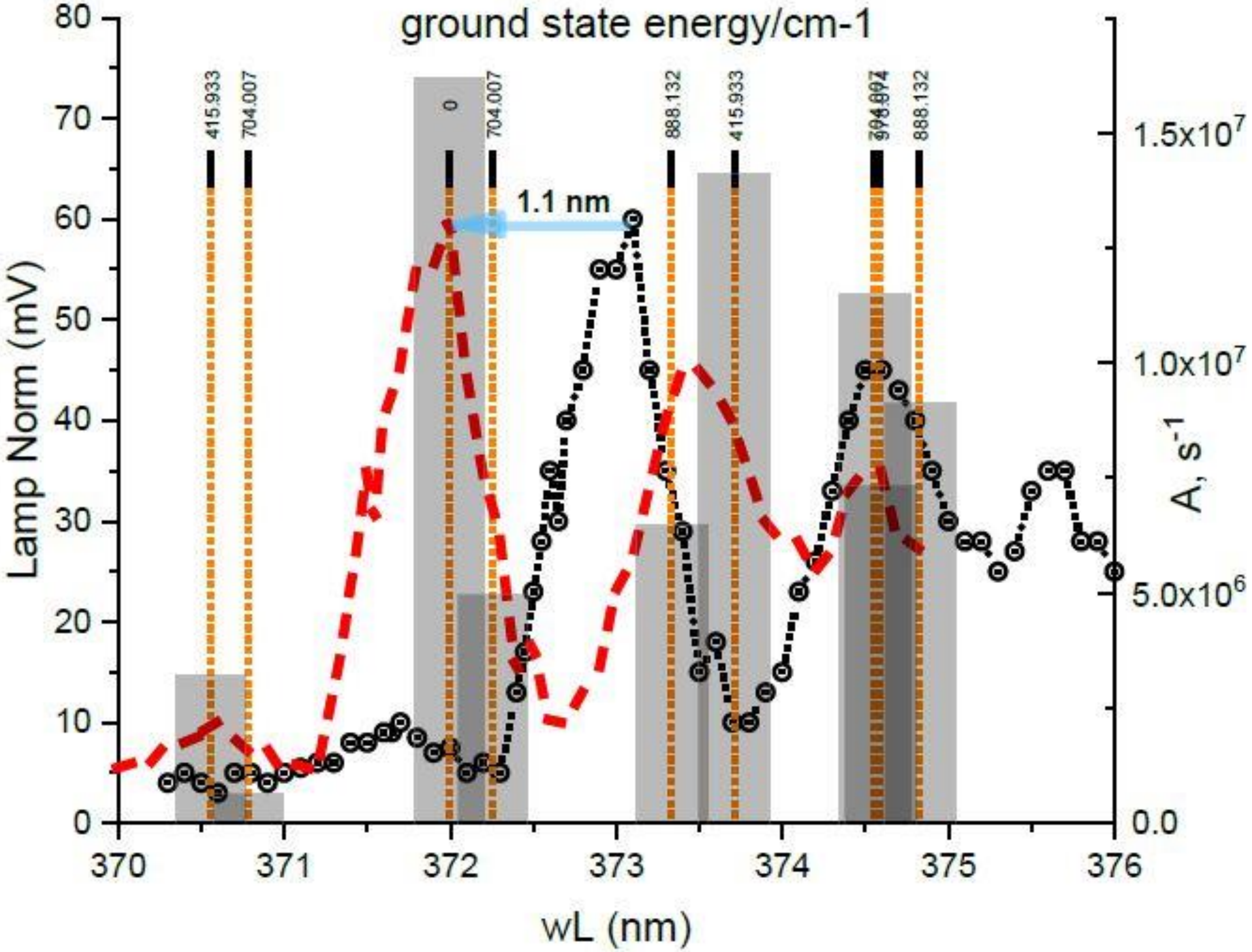




SHOCKTUBE EXPERIMENT: experimental setup for oxydation and detection of Iron

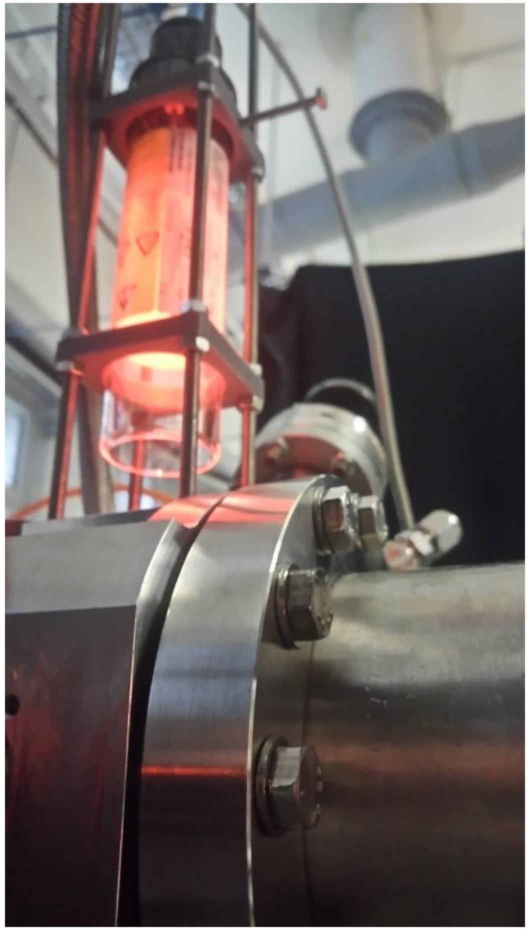
ARAS

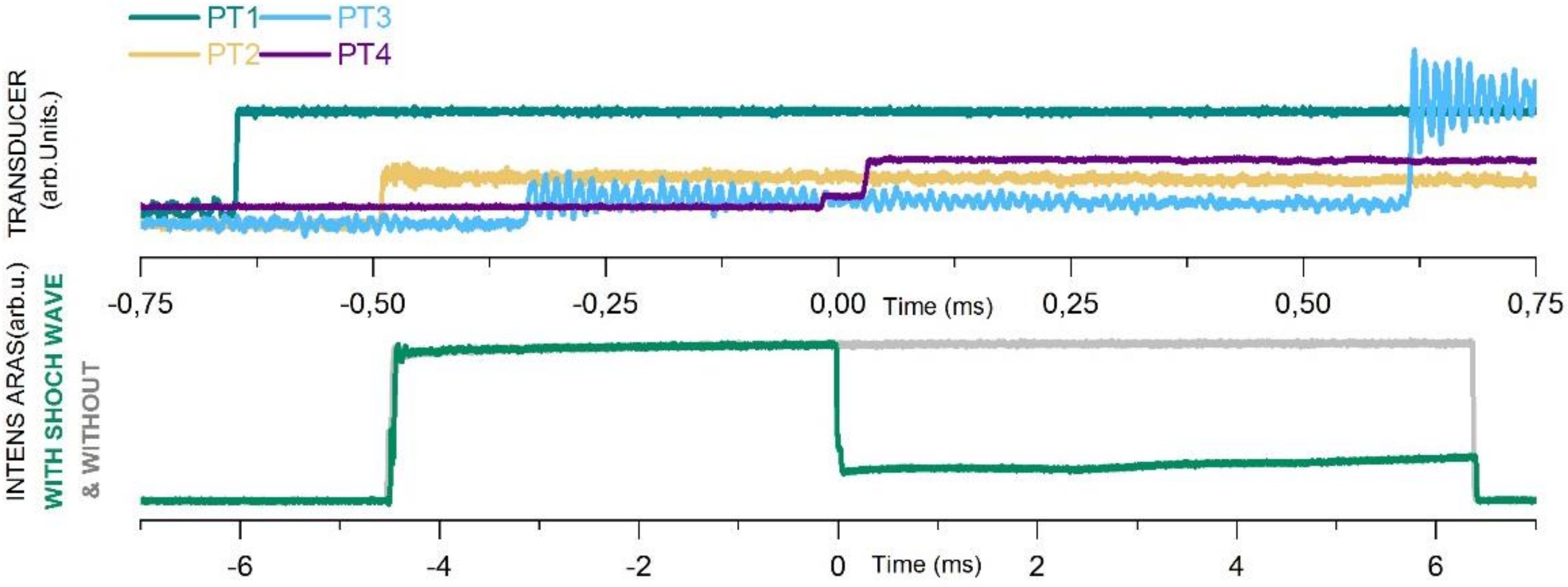




SHOCKTUBE EXPERIMENT: absorption line for detection of Iron

Shock tube & Atomic Resonance Abs. Spectroscopy (ARAS)





T and P in reflected wave from momentum and energies conservation

Software Gaseq: two dimensional secant method, (NASA method)

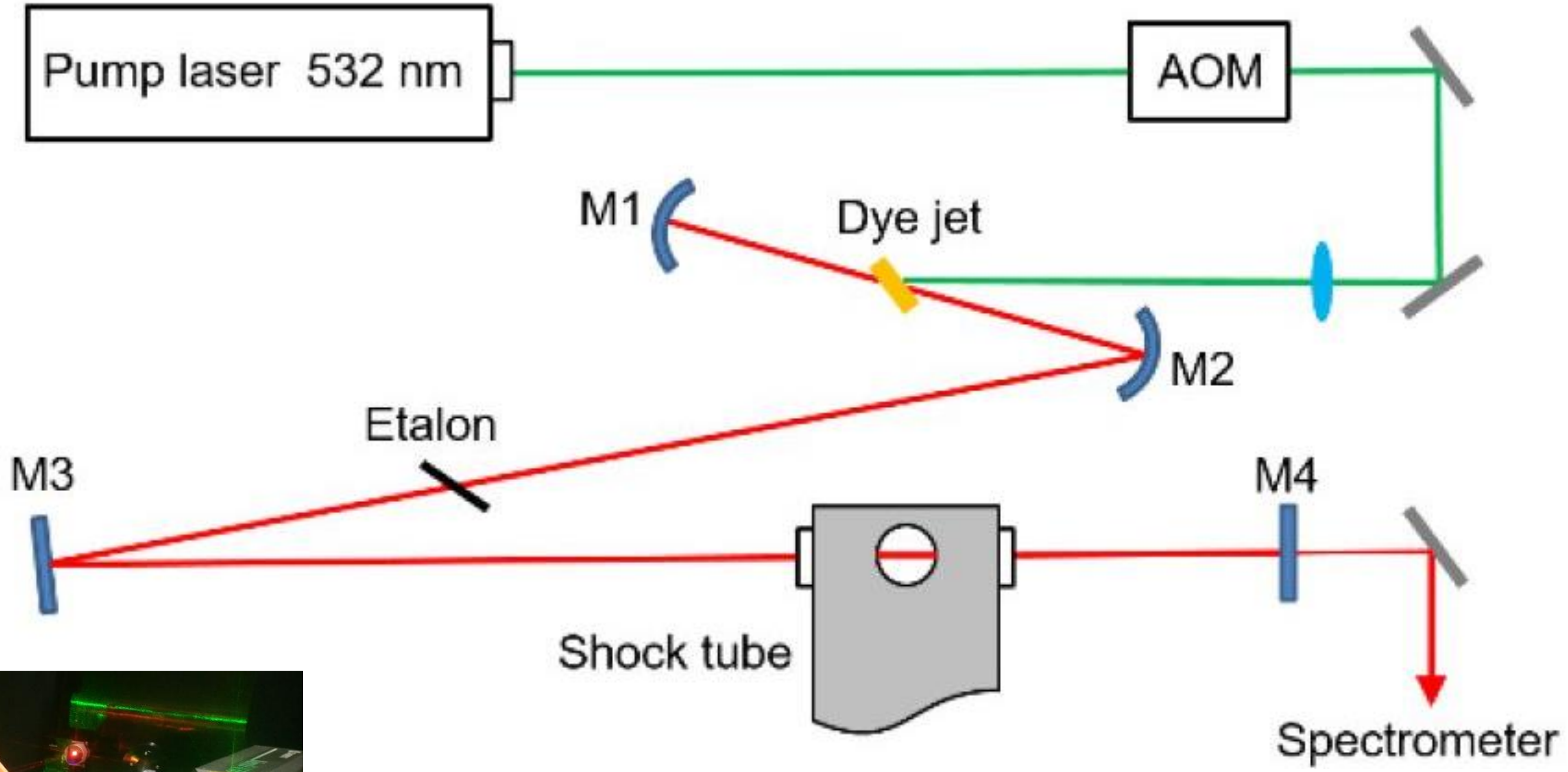
Fe quantification

Boltzman factor &Beer lambert s law

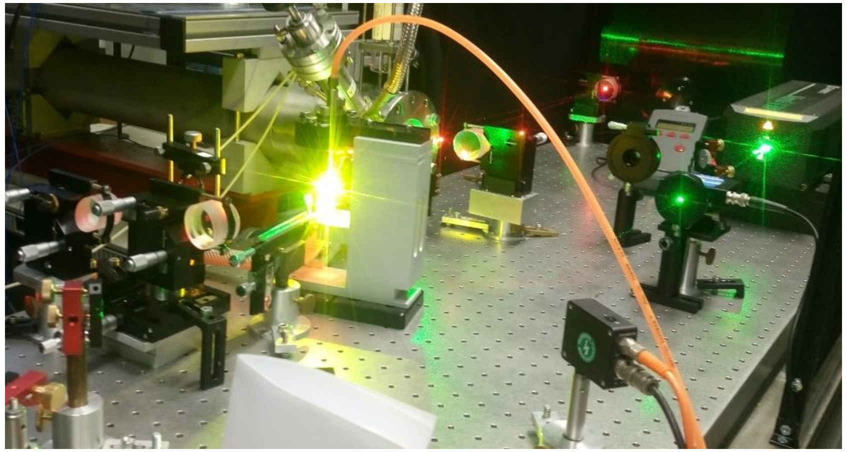
SHOCKTUBE EXPERIMENT: pressure and iron absorption time evolution

INTRA-CAVITY ABSORPTION SPECTROSCOPY (ICAS)

Verdi V10,
Coherent



Dye jet
Rhodamnine 6G
ethylene glycol



Cavity
High reflective
coated mirrors

Camera 1024 pixel
Coptronix

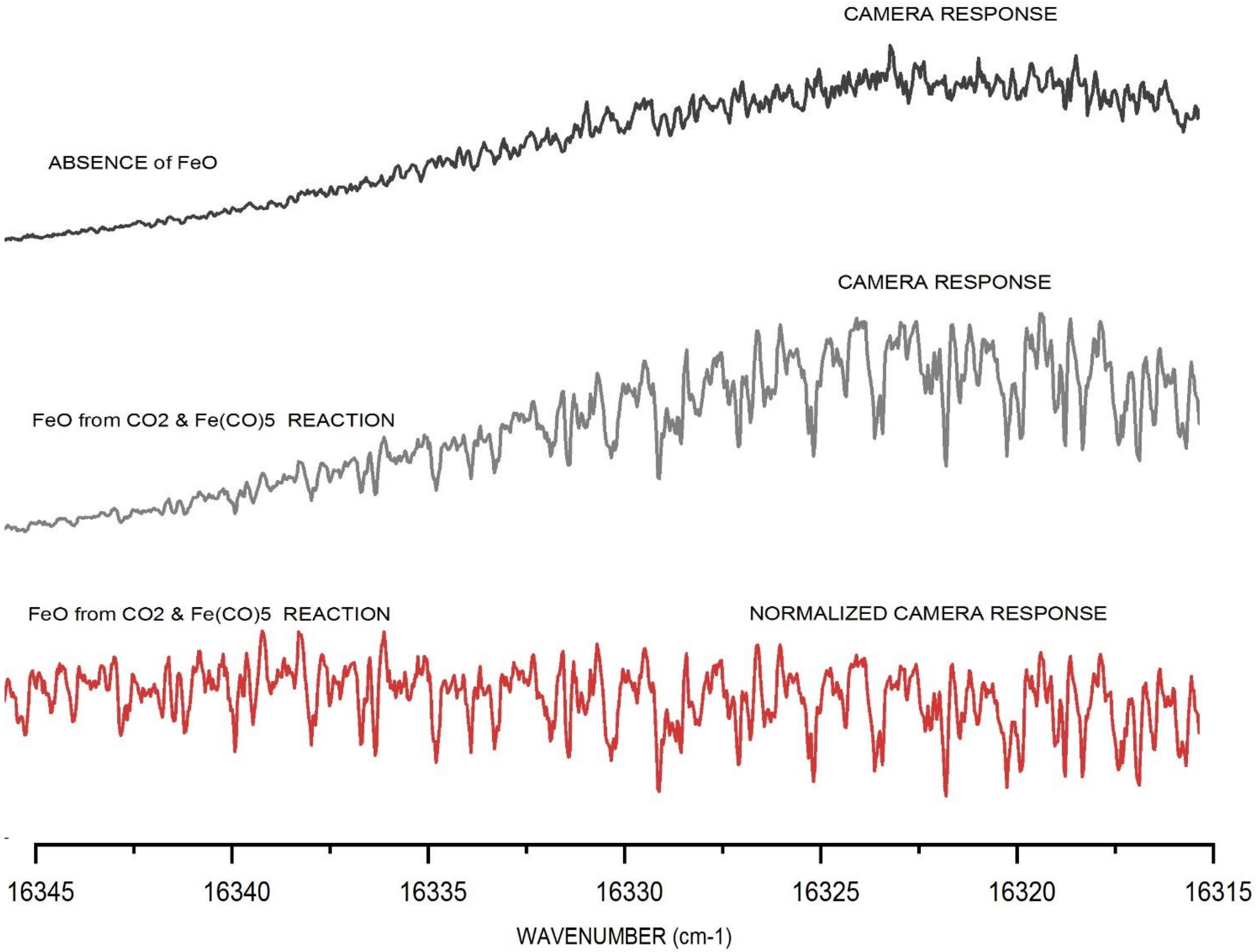
ICAS: experimental setup for FeO detection

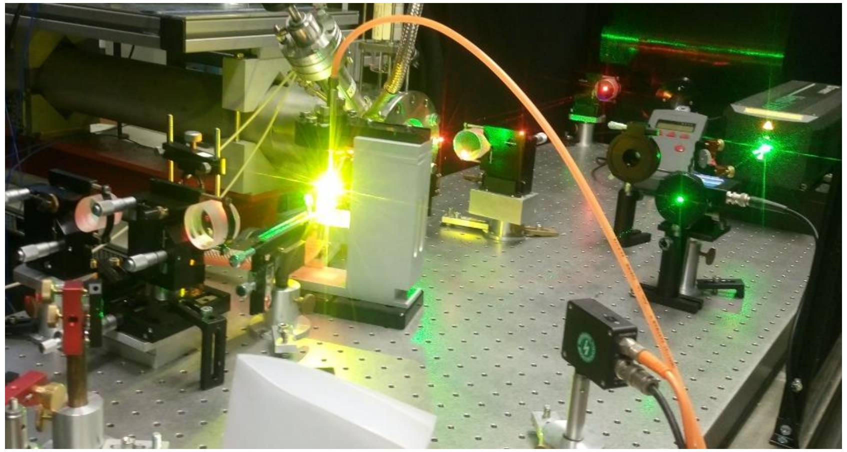
INTRA-CAVITY ABSORPTION SPECTROSCOPY (ICAS)

Muti-mode of resonce

Tunable Broadband

Band width up to 5 nm
Between 570 to 630 nm



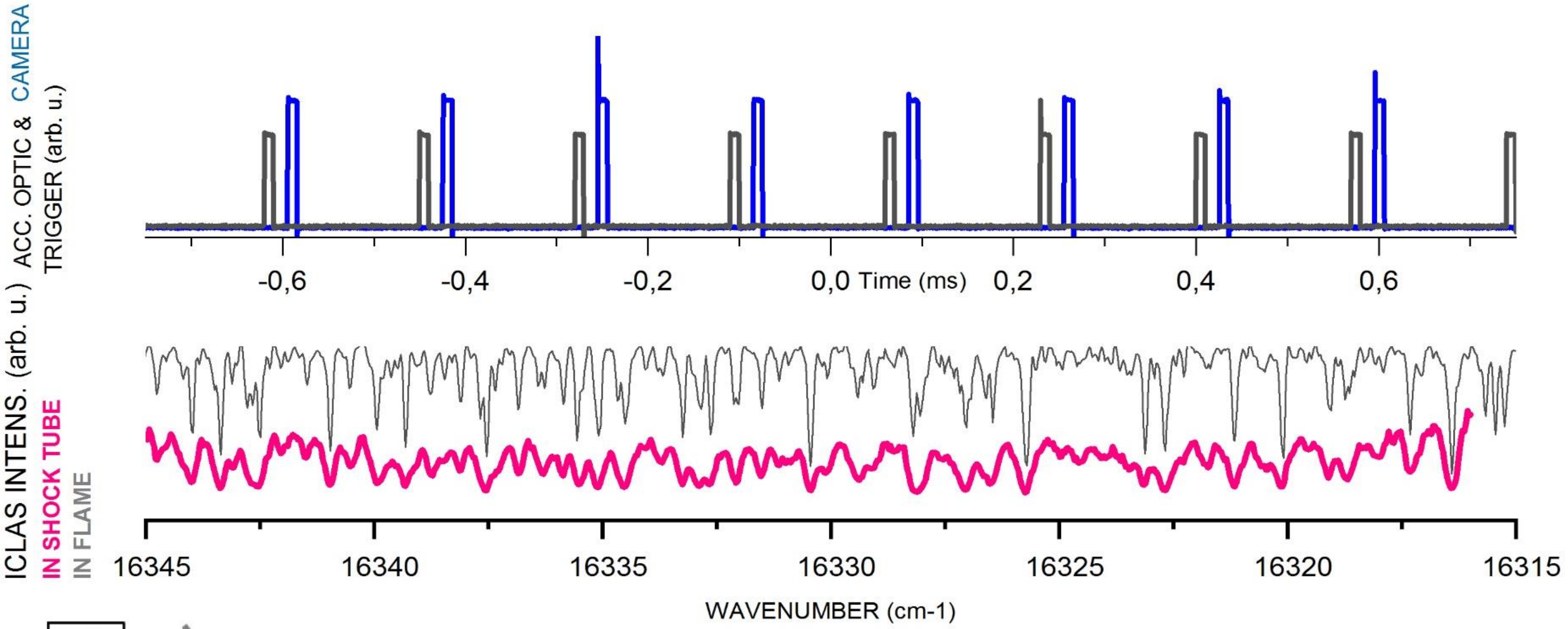


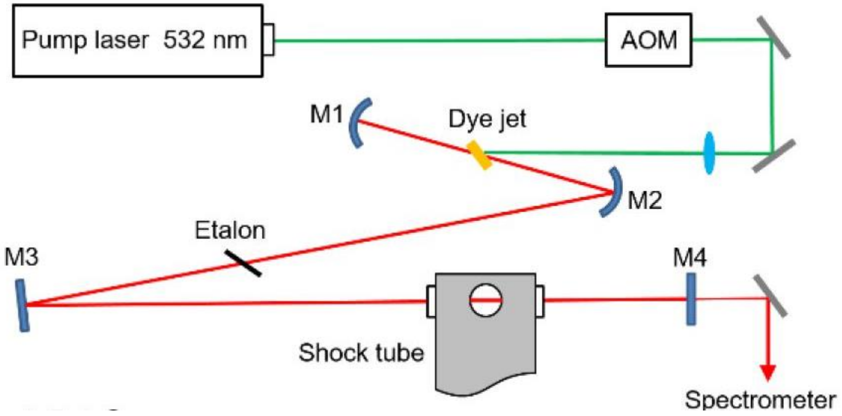
ICAS: FeO detection spectral distribution

INTRA-CAVITY ABSORPTION SPECTROSCOPY (ICAS)

Generation time
25 us

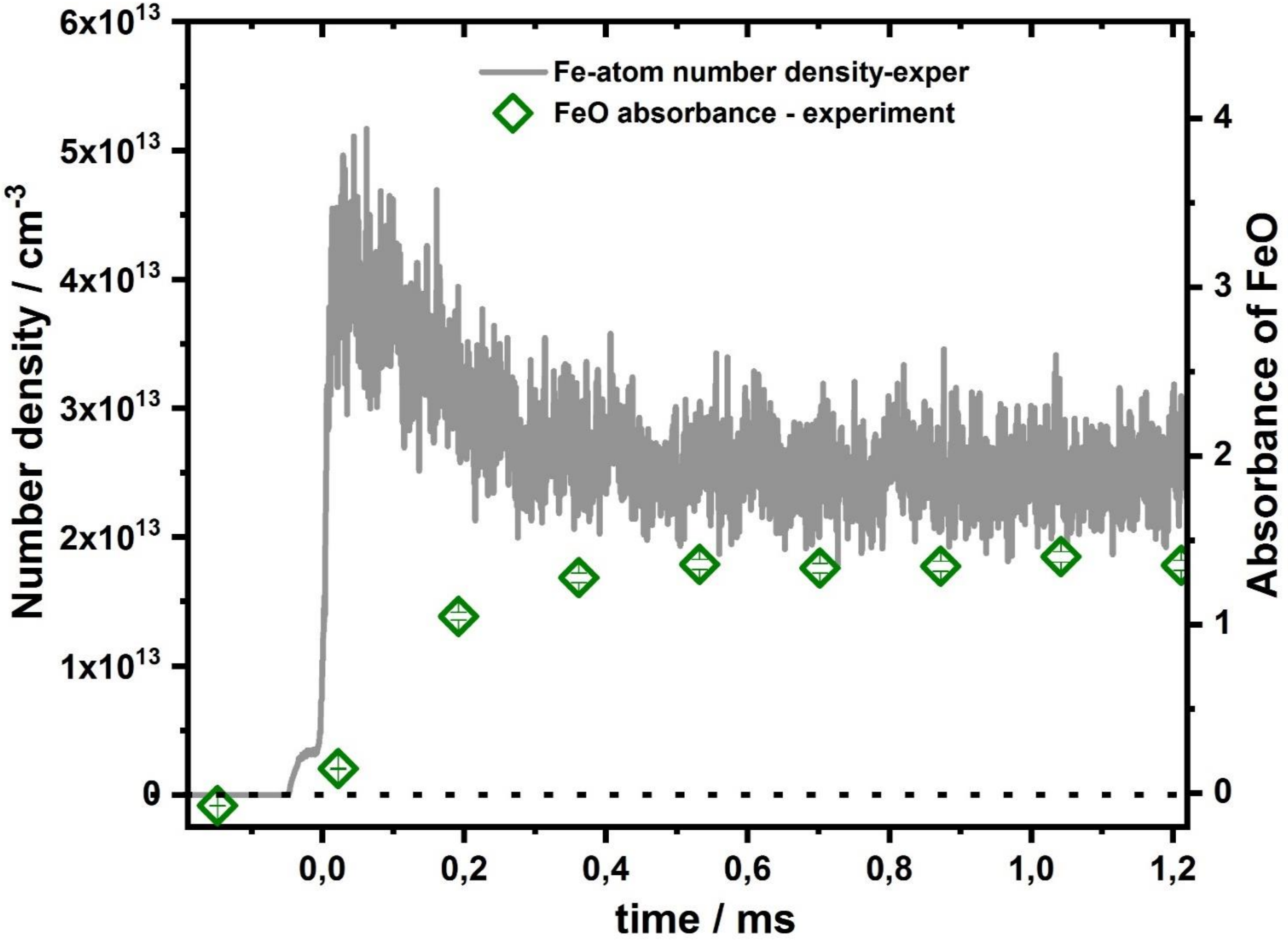
Abs. path length
280 m



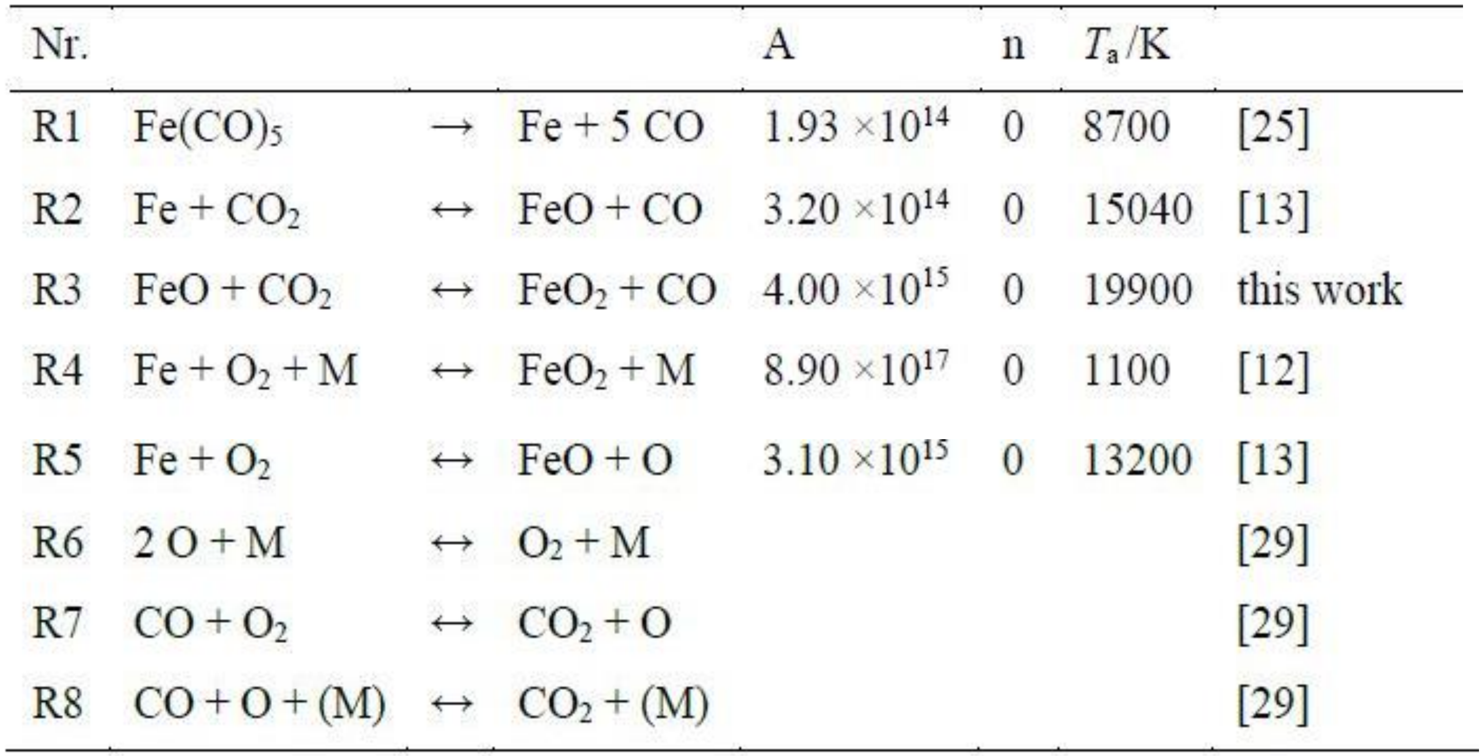


ICAS: measurement frequency and path length

ARAS & ICAS


Fe-atom number density-exper
FeO absorbance - experiment
Number density / cm^{-3}
6x10^{13}
5x10^{13}
4x10^{13}
3x10^{13}
2x10^{13}
1x10^{13}
0
Absorbance of FeO
4
3
2
1
0
0,0
0,2
0,4
0,6
0,8
1,0
1,2
time / ms

Fe & FeO

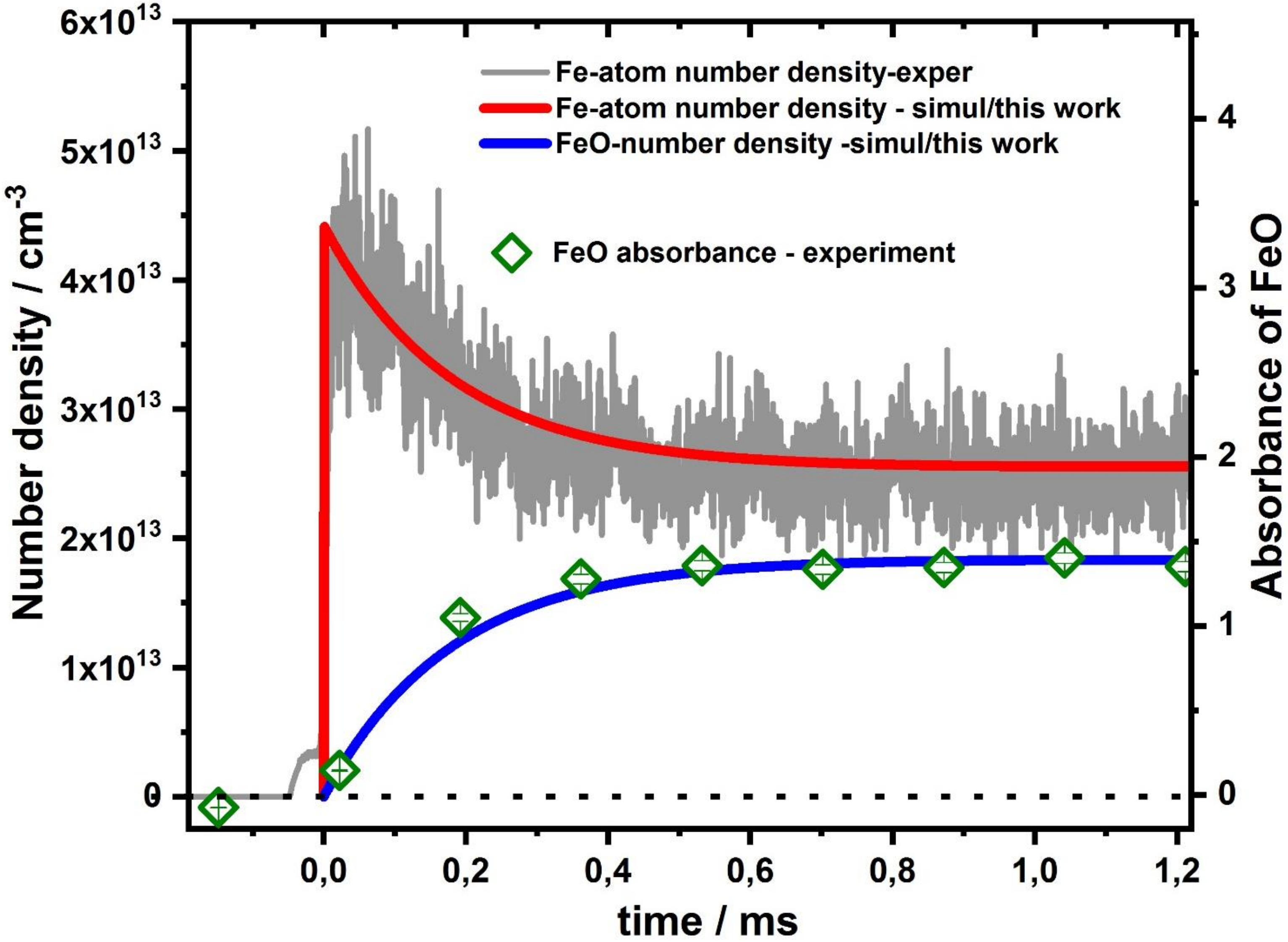


Nr.				A	n	T_a/K	
R1	$Fe(CO)_5$	→	$Fe + 5\ CO$	1.93×10^{14}	0	8700	[25]
R2	$Fe + CO_2$	↔	$FeO + CO$	3.20×10^{14}	0	15040	[13]
R3	$FeO + CO_2$	↔	$FeO_2 + CO$	4.00×10^{15}	0	19900	this work
R4	$Fe + O_2 + M$	↔	$FeO_2 + M$	8.90×10^{17}	0	1100	[12]
R5	$Fe + O_2$	↔	$FeO + O$	3.10×10^{15}	0	13200	[13]
R6	$2\ O + M$	↔	$O_2 + M$				[29]
R7	$CO + O_2$	↔	$CO_2 + O$				[29]
R8	$CO + O + (M)$	↔	$CO_2 + (M)$				[29]

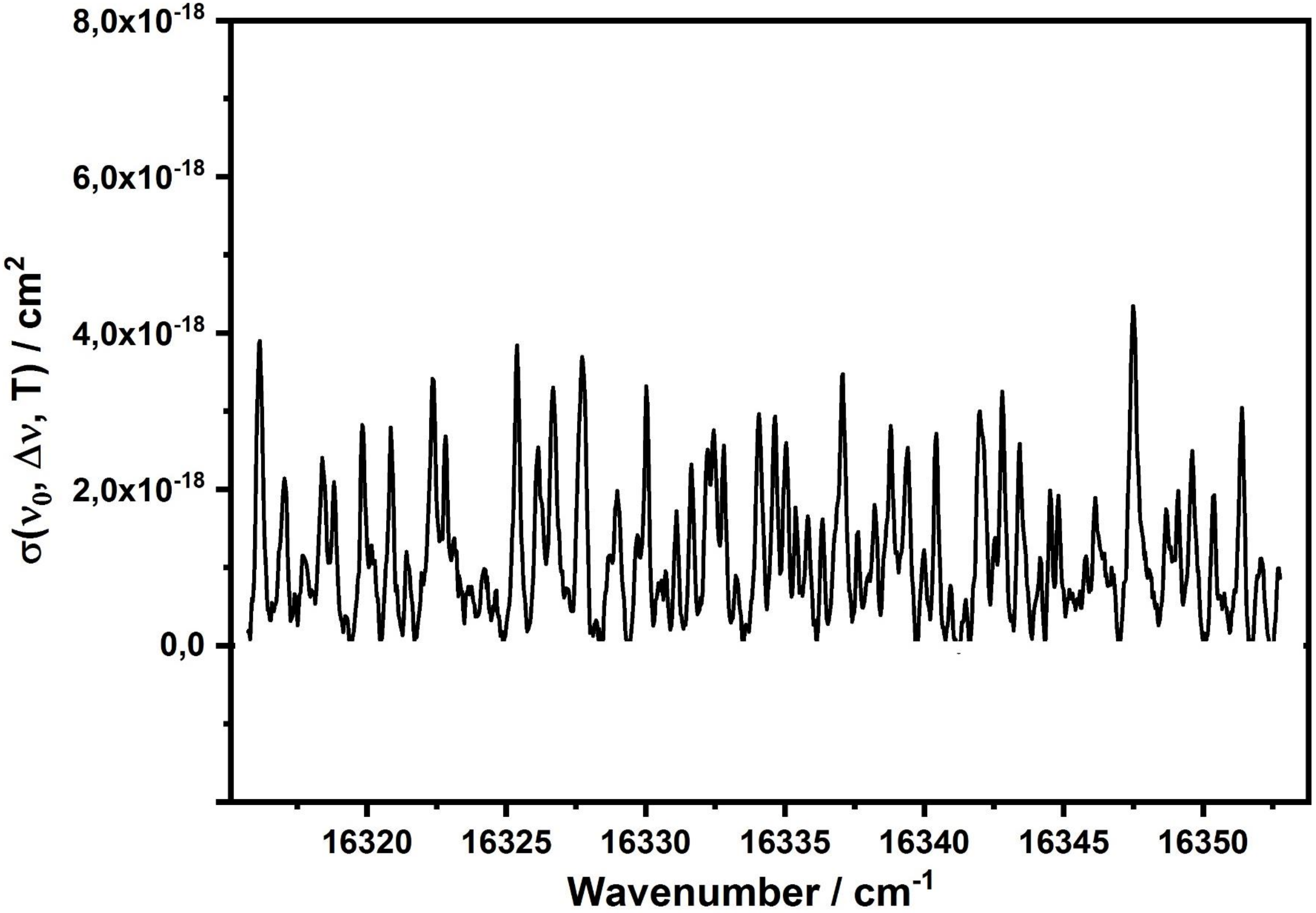
[25] Woiki et al 2001
[12] &[13] Giesen et al, 2002
[29] Varga et al,2016

[R2]: discrepancies in previous Results between Giesen et al, And Smirnov et al,

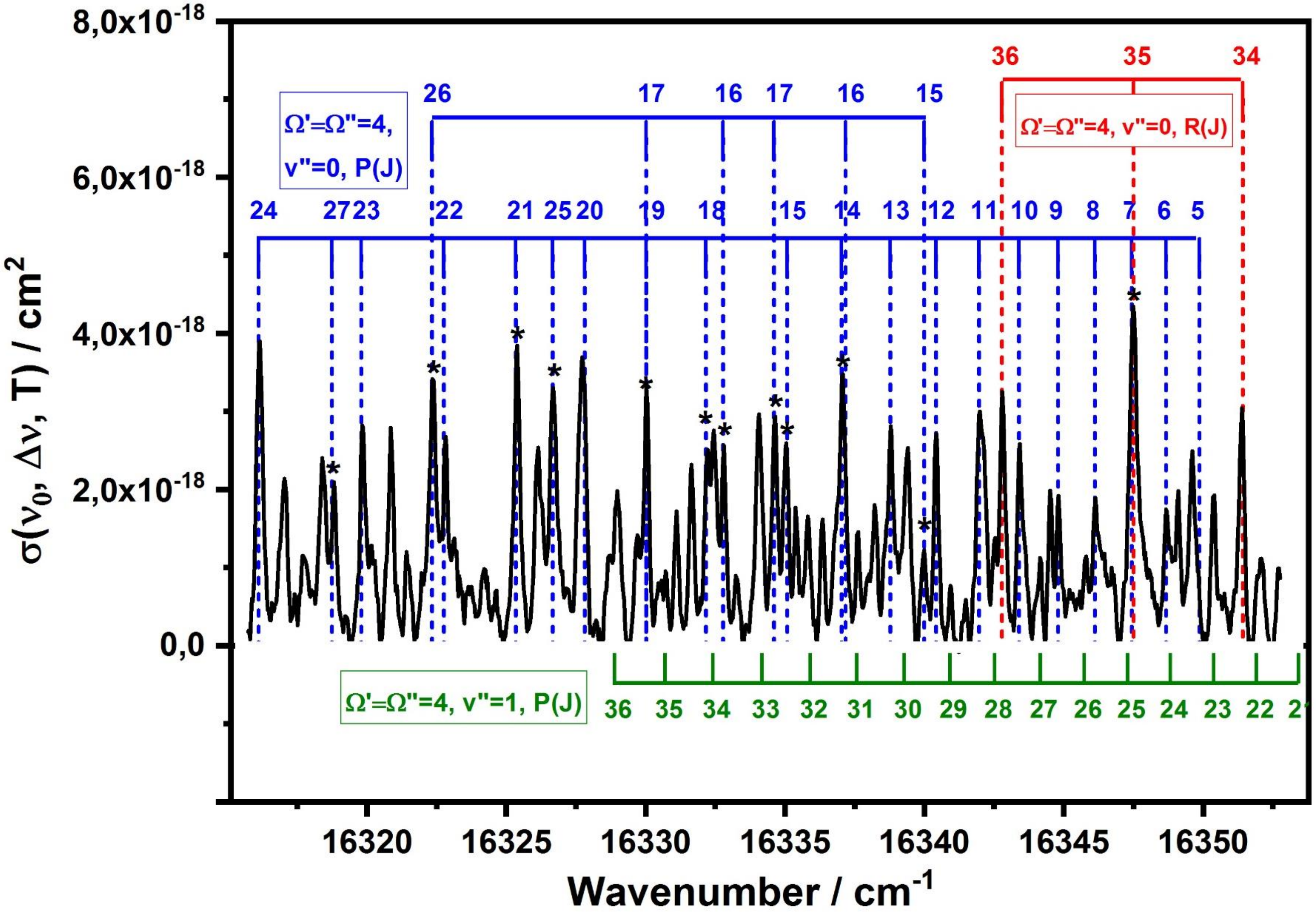
FE & FEO


Fe-atom number density-exper
Fe-atom number density - simul/this work
FeO-number density -simul/this work
FeO absorbance - experiment
Number density / cm^{-3}
Absorbance of FeO
time / ms
6x10^{13}
5x10^{13}
4x10^{13}
3x10^{13}
2x10^{13}
1x10^{13}
0
0,0
0,2
0,4
0,6
0,8
1,0
1,2
4
3
2
1
0

FeO cross Section spectrum



FeO cross Section spectrum



Ro-vibrational bands system

Cheung et al., 1983

611 nm band

$D\ ^5\Delta_4 - X\ ^5\Delta_4\ (0,0)$

Severly Perturbated
With a bond length
of 1,69A

FeO cross section & oscillator Strength

$$\int_{\text{line}} \sigma(\nu, \Delta\nu)\, d\nu = \frac{\pi e^2}{m_e c^2} f_{J'J''}$$

$$f_{J'J''} = \frac{\int_{line} \sigma(\nu, \Delta\nu, T)\, d\nu}{F_{\text{B}}(T)} \frac{m_e c^2}{\pi e^2}$$

$\sigma(\nu_0, \Delta\nu)$ the centerline absorption

$F_{\text{B}}(T)$ is the Boltzmann factor

$(\Delta\nu)$ is the spectral linewidth

$f_{J',J''}$ transition oscillator strength

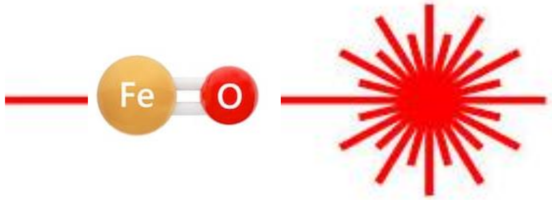
Transition	Oscillator strength, $f_{J',J''}$
P(24)	$11.4(\pm 3.0) \times 10^{-4}$
P(23)	$6.6(\pm 1.7) \times 10^{-4}$
P(12)	$9.4(\pm 2.4) \times 10^{-4}$
R(36)	$5.9(\pm 1.5) \times 10^{-4}$
R(34)	$6.4(\pm 1.7) \times 10^{-4}$

radiative lifetimes 4.7×10^3 ns to 9.7×10^3 ns.

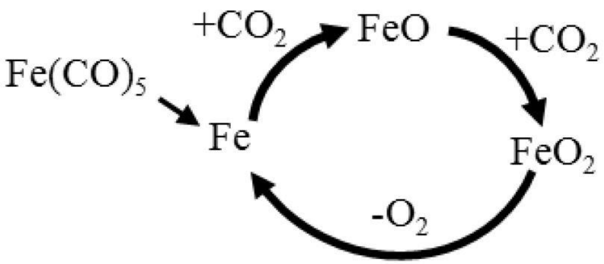
FEO ABSORPTION CROSS SECTION RESULTS: oscillator strength, a temperature independant expression

RESULTS

FeO Absorption cross section



Kinetic of FeO



Quantitative FeO investigation
in Flame and beyond

Conclusion: a small step further in determination of physical and chemical FeO behavior

AKNOWLEDGEMENT

Prof. Igor Rahinov

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Dr. Peter Fjodorow

Dr. Irenäus Wlokas

Dr. Jürgen Herzler

Dr. Monika Nanjaiah

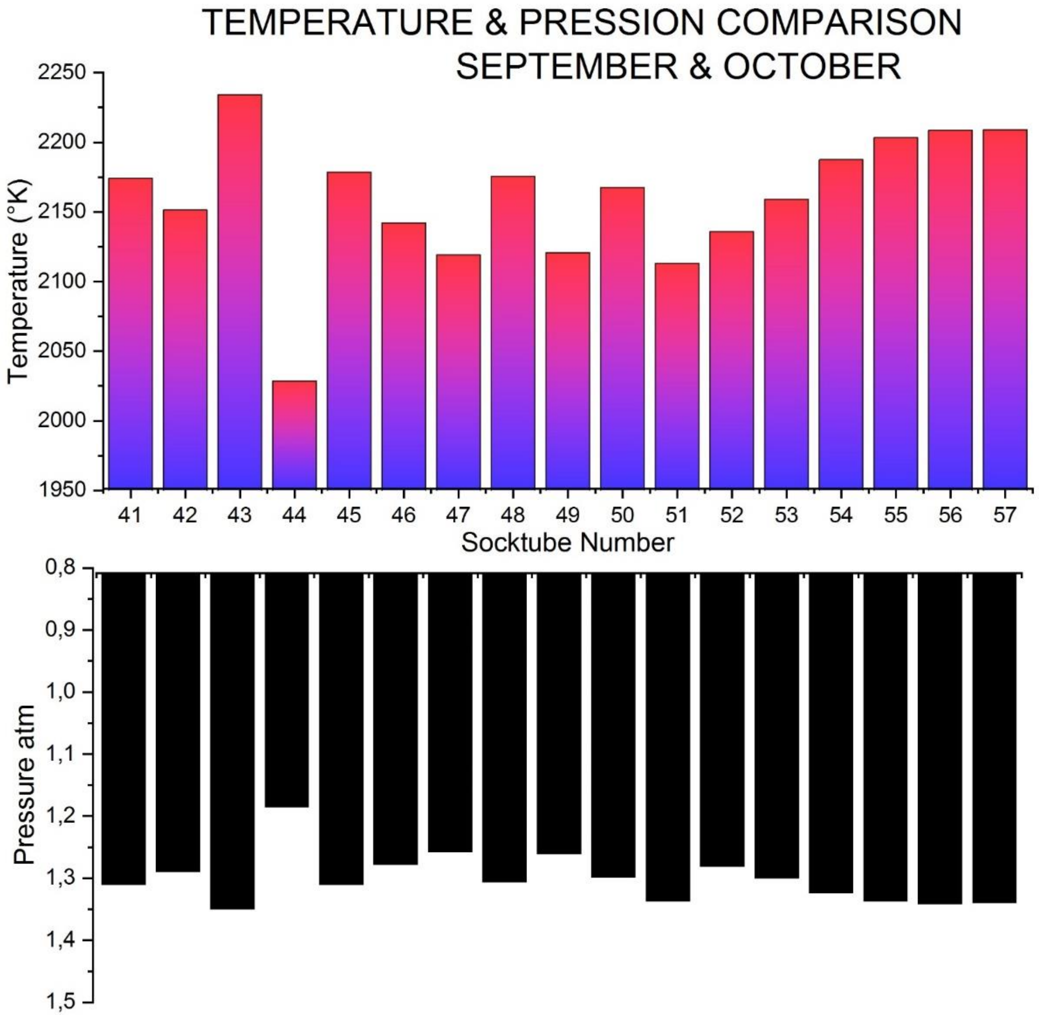
Dr. Dong He

Dr. Valery M. Baev

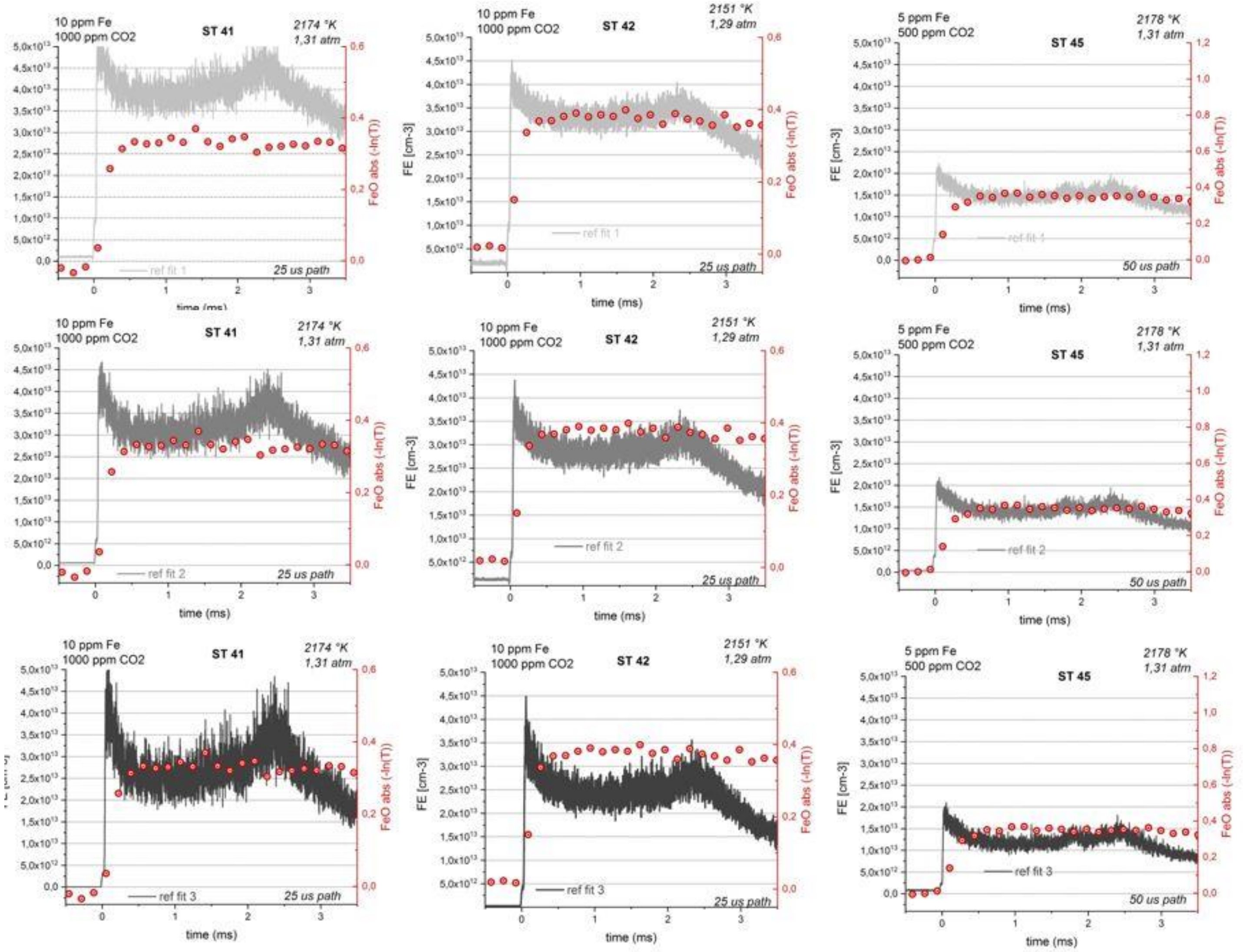
THANK YOU FOR YOUR ATTENTION

QUESTION?

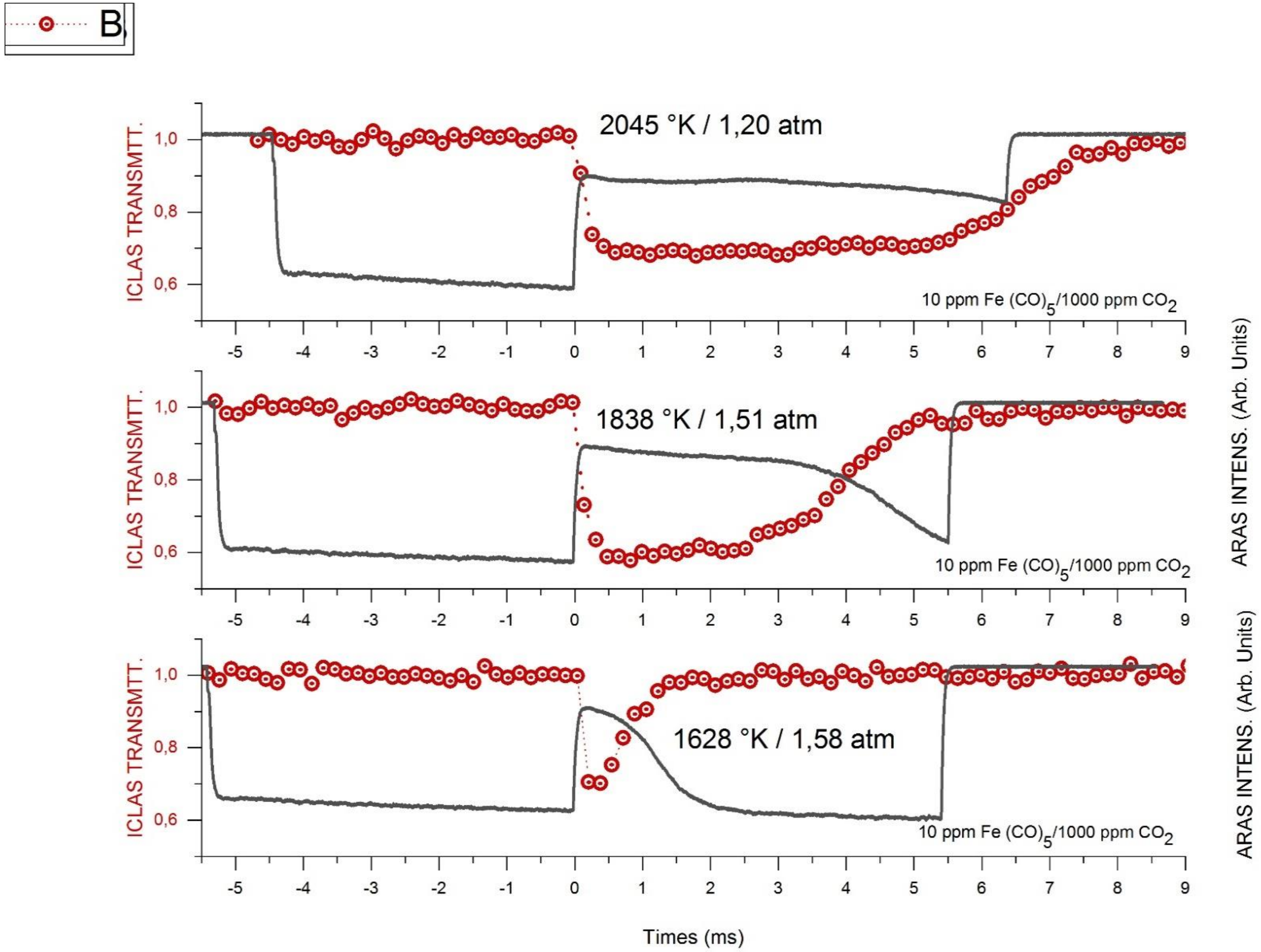
FE & FEO


TEMPERATURE & PRESSION COMPARISON
SEPTEMBER & OCTOBER
Temperature (°K)
2250
2200
2150
2100
2050
2000
1950
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
Socktube Number
Pressure atm
0,8
0,9
1,0
1,1
1,2
1,3
1,4
1,5

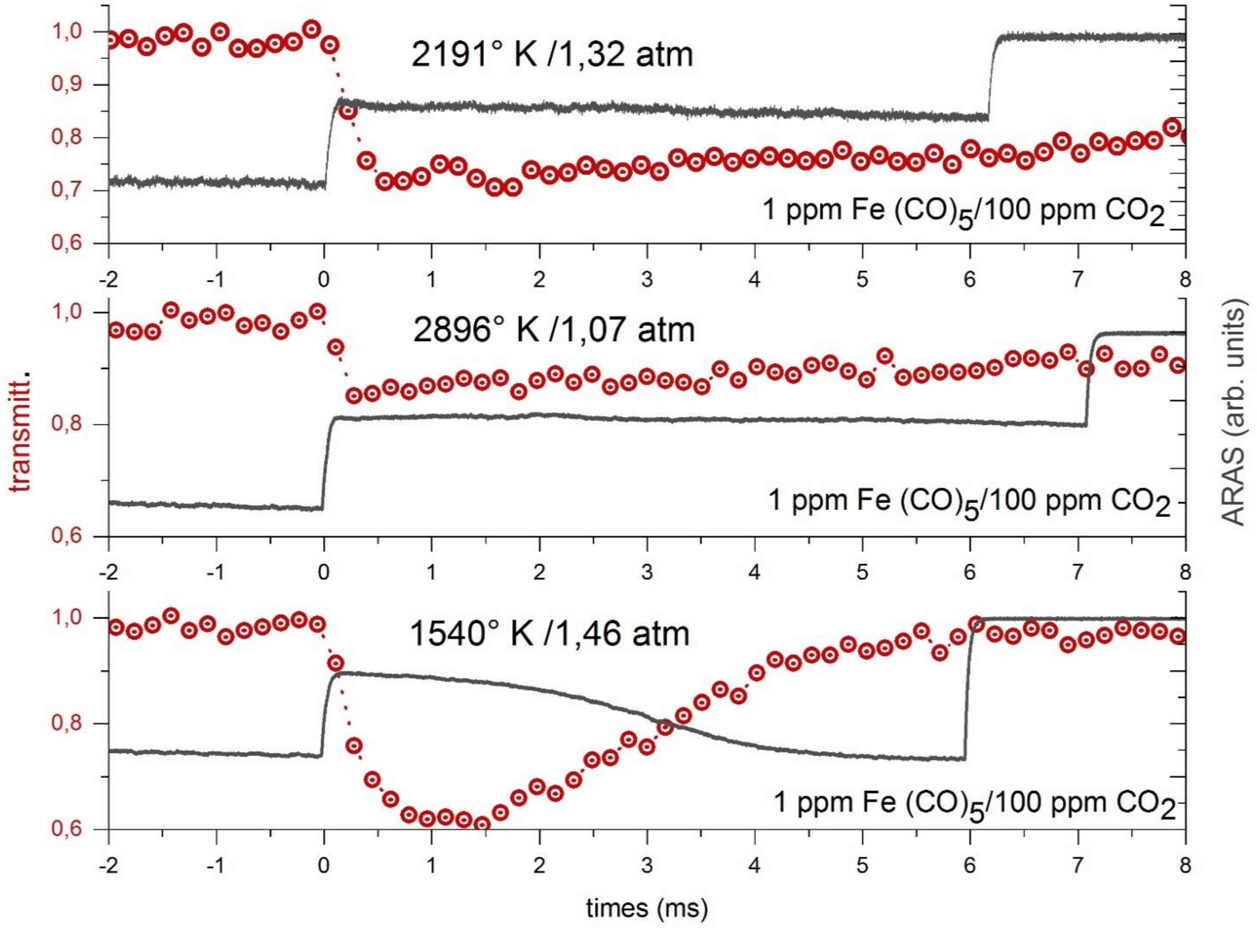
Fe & FeO


10 ppm Fe
1000 ppm CO2
ST 41
2174 °K
1,31 atm
ref fit 1
ref fit 2
ref fit 3
25 us path
10 ppm Fe
1000 ppm CO2
ST 42
2151 °K
1,29 atm
25 us path
5 ppm Fe
500 ppm CO2
ST 45
2178 °K
1,31 atm
50 us path
FE [cm-3]
FeO abs (-ln(T))
time (ms)
0,0
5,0x10^12
1,0x10^13
1,5x10^13
2,0x10^13
2,5x10^13
3,0x10^13
3,5x10^13
4,0x10^13
4,5x10^13
5,0x10^13
0,0
0,2
0,4
0,6
0,8
1,0
1,2
0
1
2
3

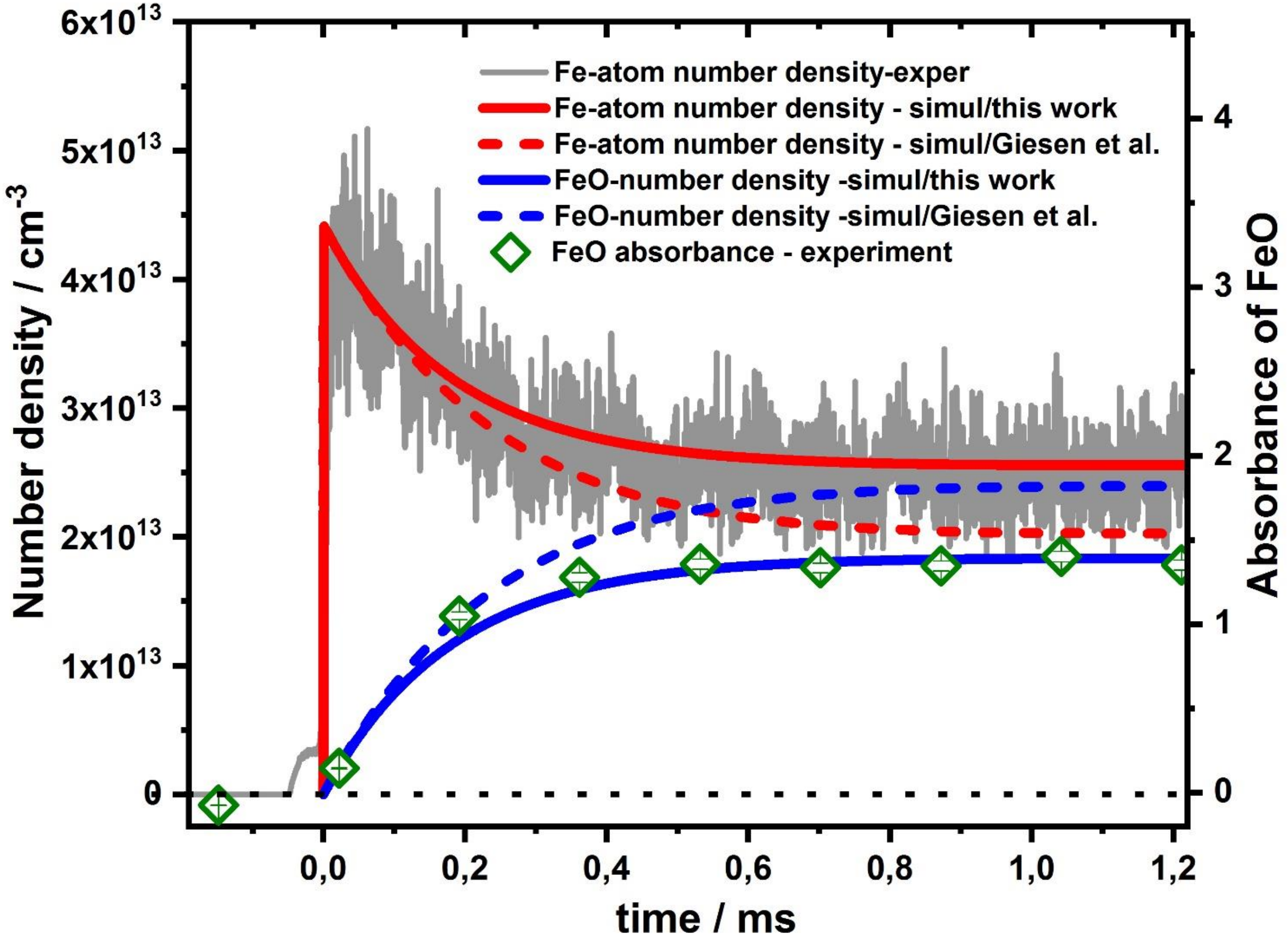
FE & FEO


B
2045 °K / 1,20 atm
1838 °K / 1,51 atm
1628 °K / 1,58 atm
10 ppm Fe (CO)$_5$/1000 ppm CO$_2$
ICLAS TRANSMTT.
ARAS INTENS. (Arb. Units)
1,0
0,8
0,6
-5
-4
-3
-2
-1
0
1
2
3
4
5
6
7
8
9
Times (ms)

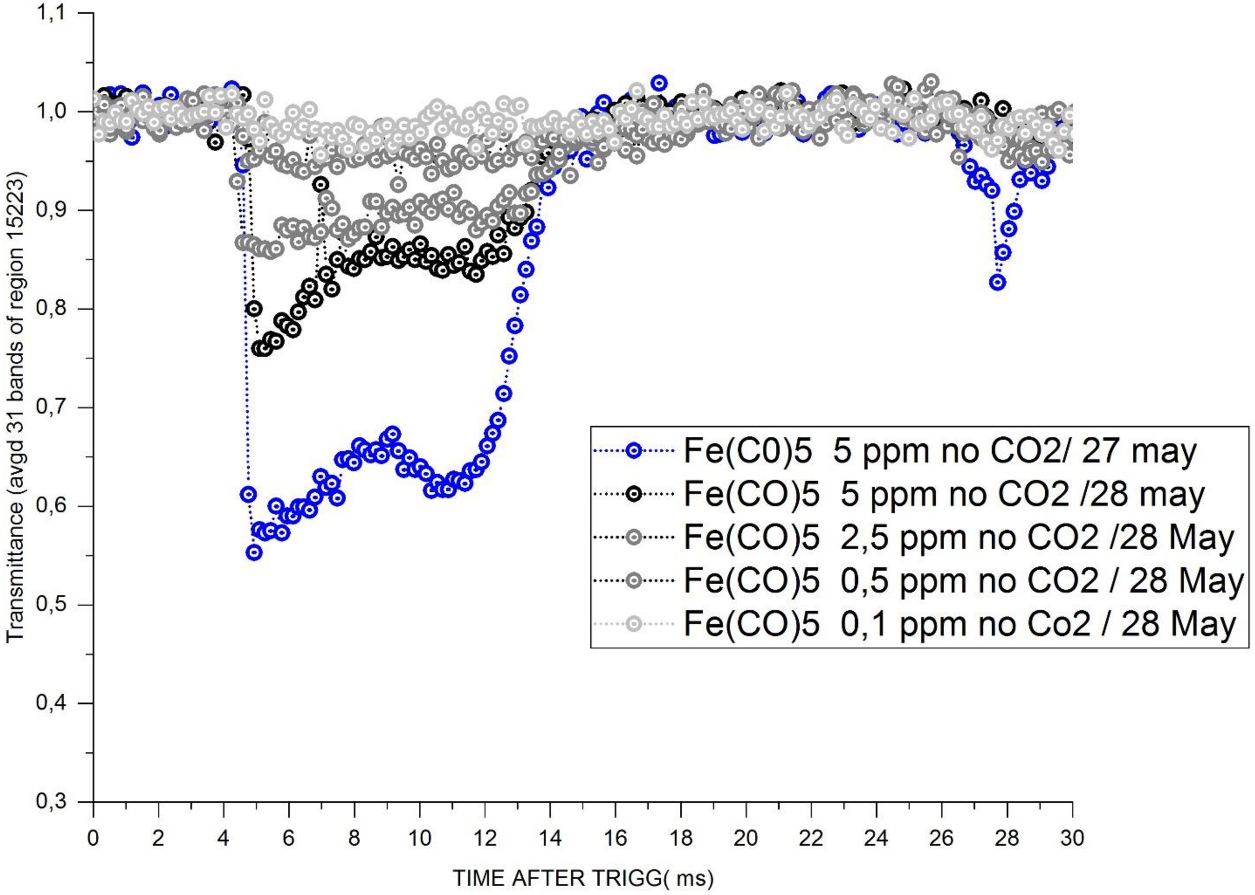
FE & FEO


2191° K /1,32 atm
1 ppm Fe (CO)$_5$/100 ppm CO$_2$
2896° K /1,07 atm
1 ppm Fe (CO)$_5$/100 ppm CO$_2$
1540° K /1,46 atm
1 ppm Fe (CO)$_5$/100 ppm CO$_2$
transmitt.
ARAS (arb. units)
times (ms)
1,0
0,9
0,8
0,7
0,6
-2
-1
0
1
2
3
4
5
6
7
8

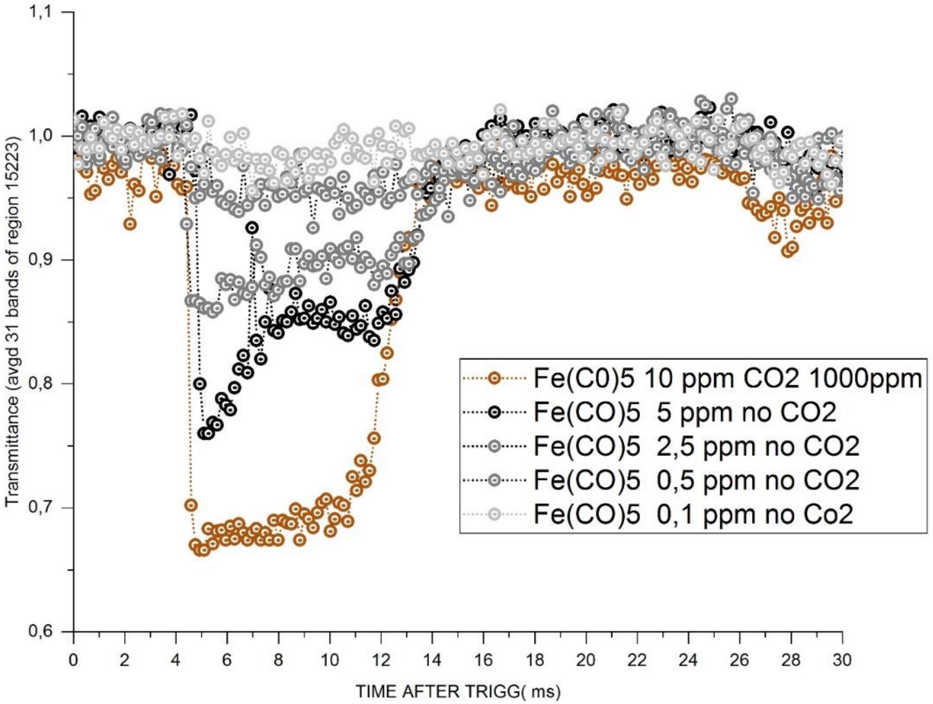
FE & FEO

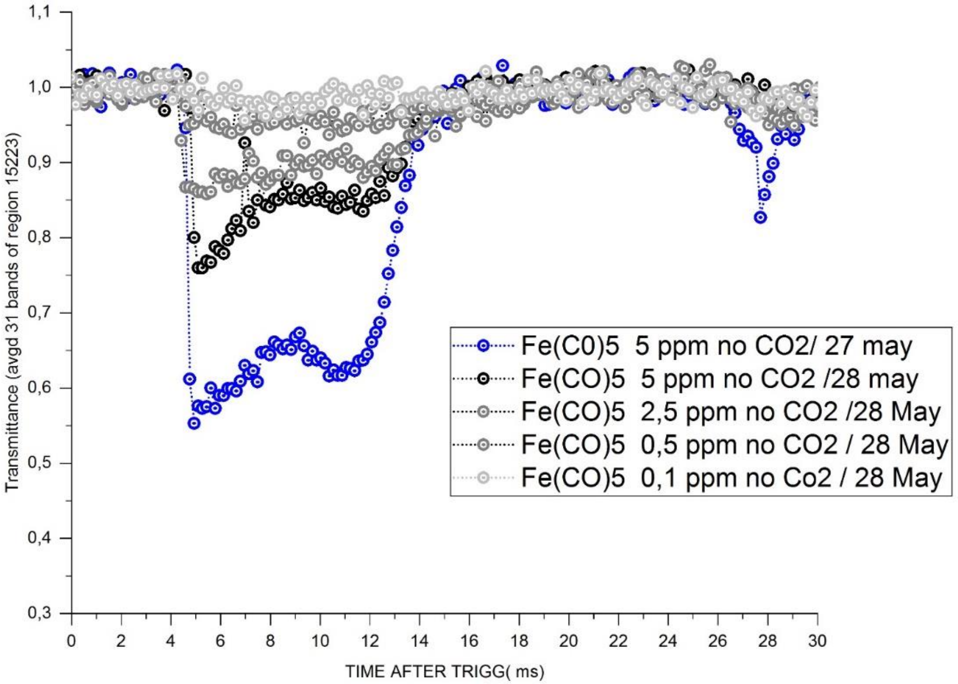

Fe-atom number density-exper
Fe-atom number density - simul/this work
Fe-atom number density - simul/Giesen et al.
FeO-number density -simul/this work
FeO-number density -simul/Giesen et al.
FeO absorbance - experiment
Number density / cm^{-3}
6x10^{13}
5x10^{13}
4x10^{13}
3x10^{13}
2x10^{13}
1x10^{13}
0
Absorbance of FeO
4
3
2
1
0
0,0
0,2
0,4
0,6
0,8
1,0
1,2
time / ms

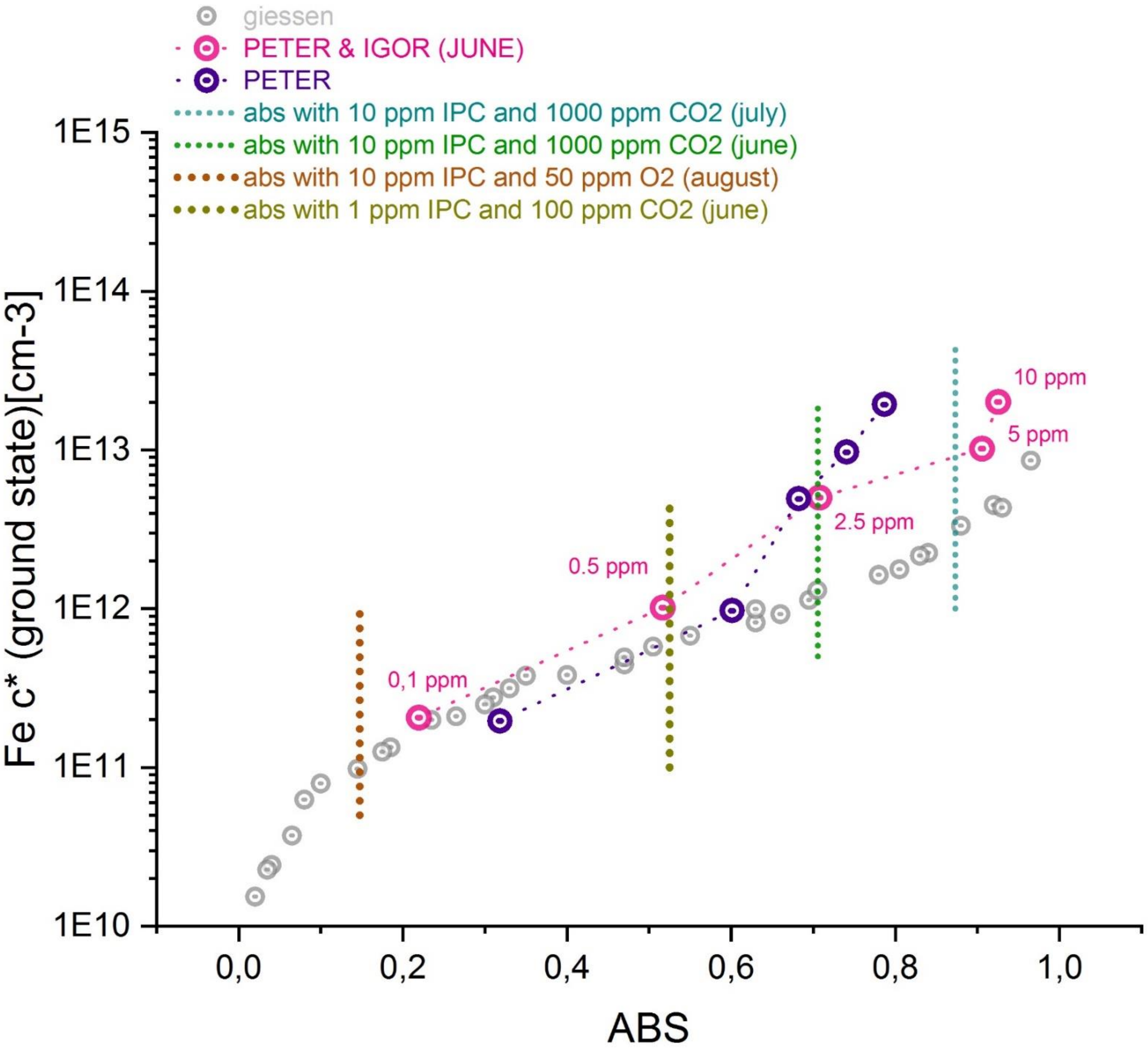
Fe & FeO

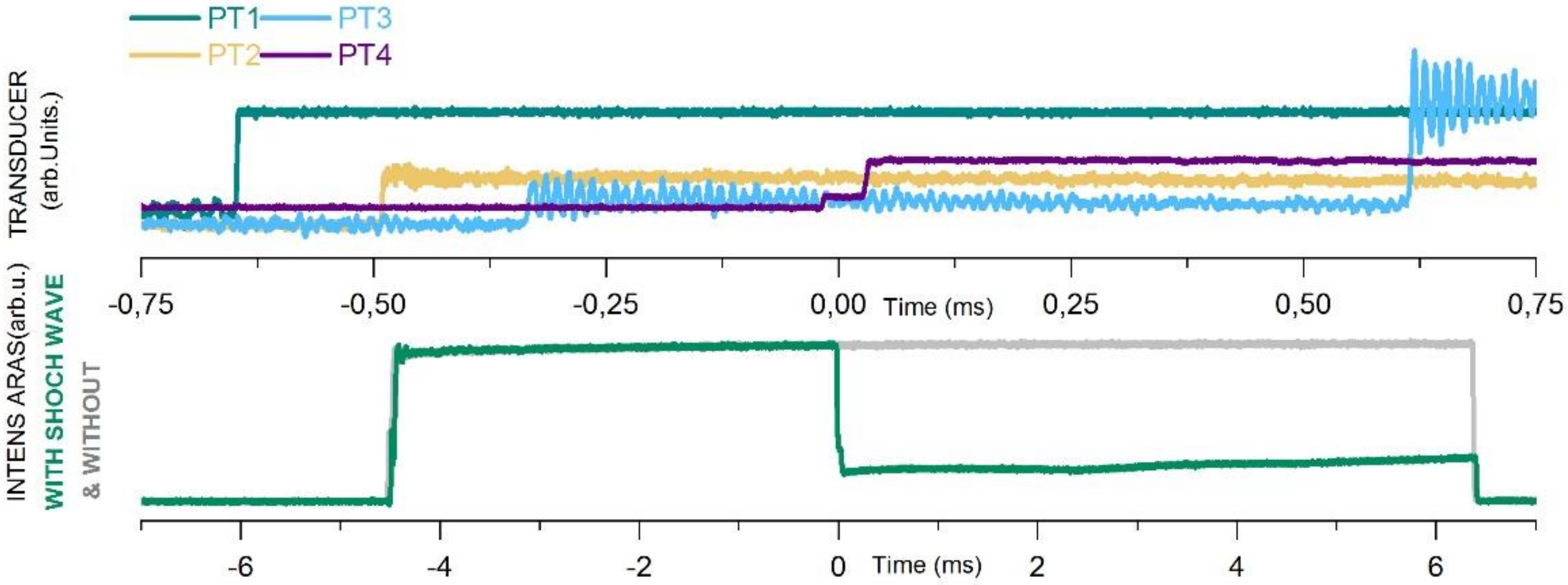

1,1
1,0
0,9
0,8
0,7
0,6
0,5
0,4
0,3
Transmittance (avgd 31 bands of region 15223)
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
TIME AFTER TRIGG(ms)
Fe(C0)5 5 ppm no CO2/ 27 may
Fe(CO)5 5 ppm no CO2 /28 may
Fe(CO)5 2,5 ppm no CO2 /28 May
Fe(CO)5 0,5 ppm no CO2 / 28 May
Fe(CO)5 0,1 ppm no Co2 / 28 May

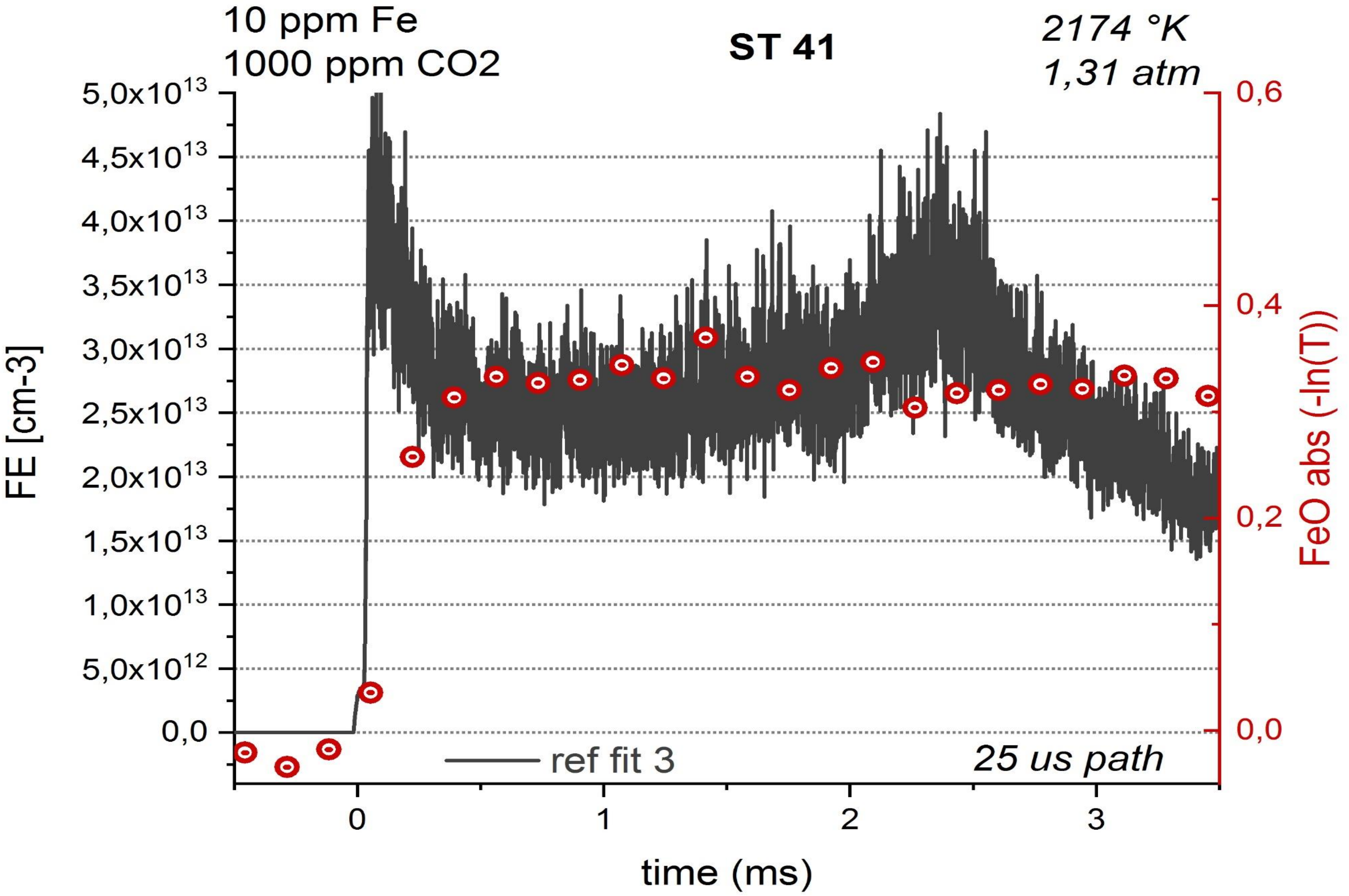
Fe & FeO


1,1
1,0
0,9
0,8
0,7
0,6
Transmittance (avgd 31 bands of region 15223)
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
TIME AFTER TRIGG(ms)
Fe(C0)5 10 ppm CO2 1000ppm
Fe(CO)5 5 ppm no CO2
Fe(CO)5 2,5 ppm no CO2
Fe(CO)5 0,5 ppm no CO2
Fe(CO)5 0,1 ppm no Co2


1,1
1,0
0,9
0,8
0,7
0,6
0,5
0,4
0,3
Transmittance (avgd 31 bands of region 15223)
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
TIME AFTER TRIGG(ms)
Fe(C0)5 5 ppm no CO2/ 27 may
Fe(CO)5 5 ppm no CO2 /28 may
Fe(CO)5 2,5 ppm no CO2 /28 May
Fe(CO)5 0,5 ppm no CO2 / 28 May
Fe(CO)5 0,1 ppm no Co2 / 28 May


giessen
PETER & IGOR (JUNE)
PETER
abs with 10 ppm IPC and 1000 ppm CO2 (july)
abs with 10 ppm IPC and 1000 ppm CO2 (june)
abs with 10 ppm IPC and 50 ppm O2 (august)
abs with 1 ppm IPC and 100 ppm CO2 (june)
Fe c* (ground state)[cm-3]
1E15
1E14
1E13
1E12
1E11
1E10
10 ppm
5 ppm
2.5 ppm
0.5 ppm
0,1 ppm
0,0
0,2
0,4
0,6
0,8
1,0
ABS


PT1
PT3
PT2
PT4
TRANSDUCER (arb.Units.)
-0,75
-0,50
-0,25
0,00
Time (ms)
0,25
0,50
0,75
INTENS ARAS(arb.u.)
WITH SHOCH WAVE
& WITHOUT
-6
-4
-2
0
Time (ms)
2
4
6


10 ppm Fe
1000 ppm CO2
ST 41
2174 °K
1,31 atm
FE [cm-3]
5,0x10^13
4,5x10^13
4,0x10^13
3,5x10^13
3,0x10^13
2,5x10^13
2,0x10^13
1,5x10^13
1,0x10^13
5,0x10^12
0,0
FeO abs (-ln(T))
0,6
0,4
0,2
0,0
ref fit 3
25 us path
0
1
2
3
time (ms)

Nr.				A	n	T_a /K	
R1	$Fe(CO)_5$	→	Fe + 5 CO	1.93×10^{14}	0	8700	[25]
R2	$Fe + CO_2$	↔	FeO + CO	3.20×10^{14}	0	15040	[13]
R3	$FeO + CO_2$	↔	$FeO_2 + CO$	4.00×10^{15}	0	19900	this work
R4	$Fe + O_2 + M$	↔	$FeO_2 + M$	8.90×10^{17}	0	1100	[12]
R5	$Fe + O_2$	↔	FeO + O	3.10×10^{15}	0	13200	[13]
R6	2 O + M	↔	$O_2 + M$				[29]
R7	$CO + O_2$	↔	$CO_2 + O$				[29]
R8	CO + O + (M)	↔	CO_2 + (M)				[29]

Shocks and Detonations

A two dimensional secant method is used ("Data reduction and analysis", p234). The variables P_2 and T_2 are adjusted until the following functions are zero. (These are the basic energy and momentum conservation equations.)

$$P_1 - P_2 + \rho_1 u_1^2 - \rho_2 u_2^2 = 0$$
$$h_1 - h_2 + 0.5(u_1^2 - u_2^2) = 0$$

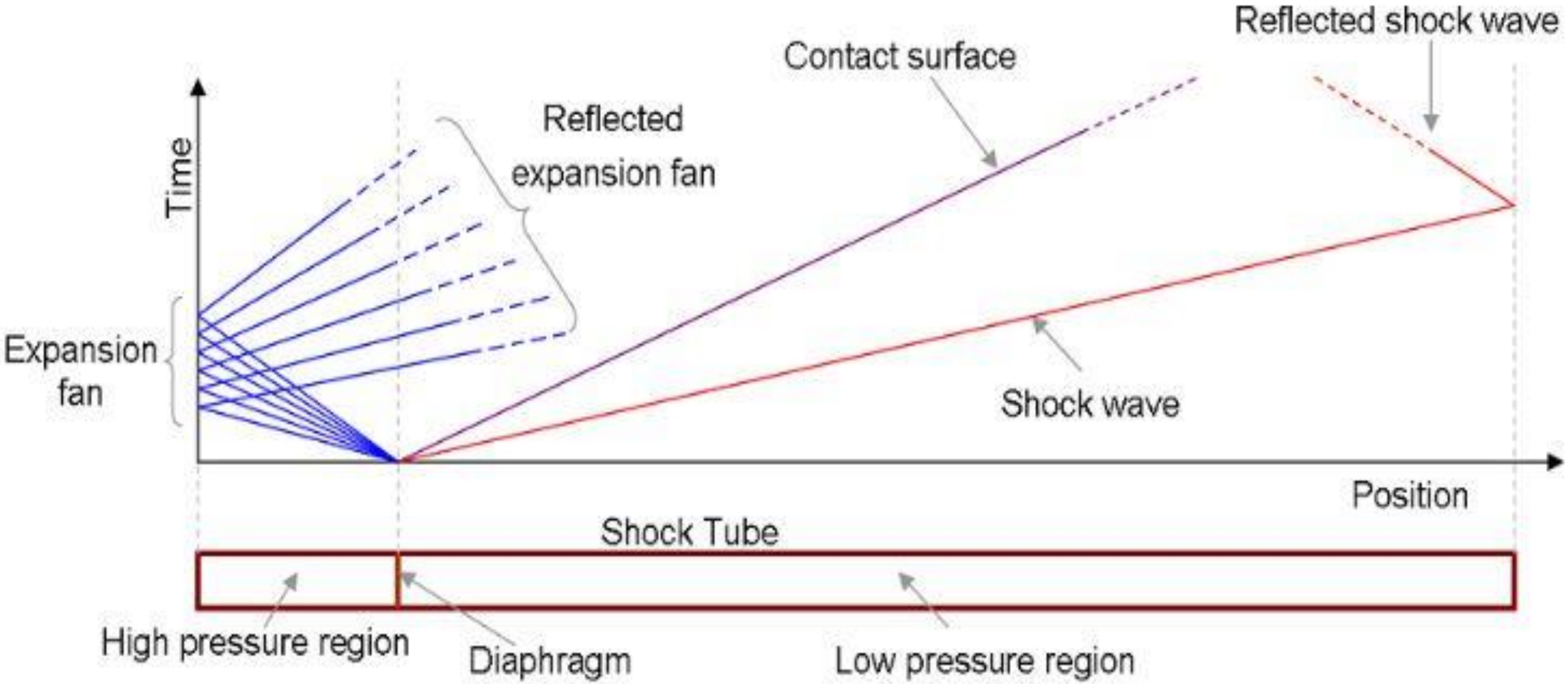
The subscripts 1 and 2 are before and after the shock respectively. The *h*'s are enthalpies and the ρ's are densities. The *u*'s are gas velocities relative to the shock and are obtained in different ways for incident, reflected and C-J detonation calculations.

For incident shocks the shock speed relative to the stationary gas ahead of the shock is u_1, and continuity gives

$$u_2 = u_1 \rho_1 / \rho_2$$

For reflected shocks, an incident shock calculation is done first and the gas velocity in lab coordinates after the incident shock, v_S used:

$$u_2 = \frac{\rho_1 v_S}{\rho_2 - \rho_1}$$
$$u_1 = u_2 + v_S$$

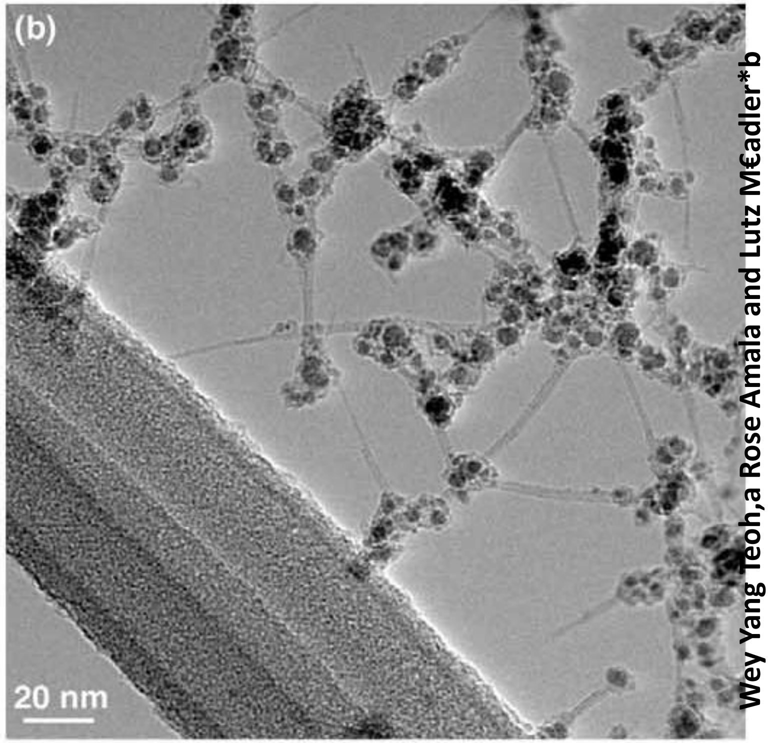

Reflected shock wave
Contact surface
Reflected expansion fan
Time
Expansion fan
Shock wave
Position
Shock Tube
High pressure region
Diaphragm
Low pressure region

FLAME MADE MATERIAL

>$ 15 Billions/ yr

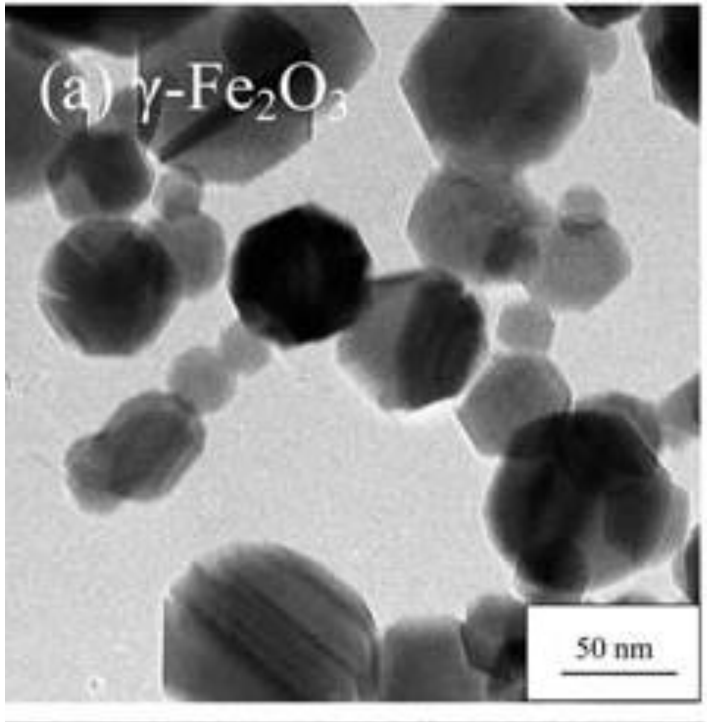
Li-doped Na$_2$O.xA$_{l2}$O$_3$
Li-ZnO
LiMnO$_4$
Borosilicate glass
BaCO$_3$

RANDALL L. VANDER WAL* and LEE J. HALL*COMBUSTION AND FLAME* 130:27–36 (2002



MgO-Fe$_2$O$_3$
MgO-Al$_2$O$_3$
3Al$_2$O$_3$.2SiO$_2$

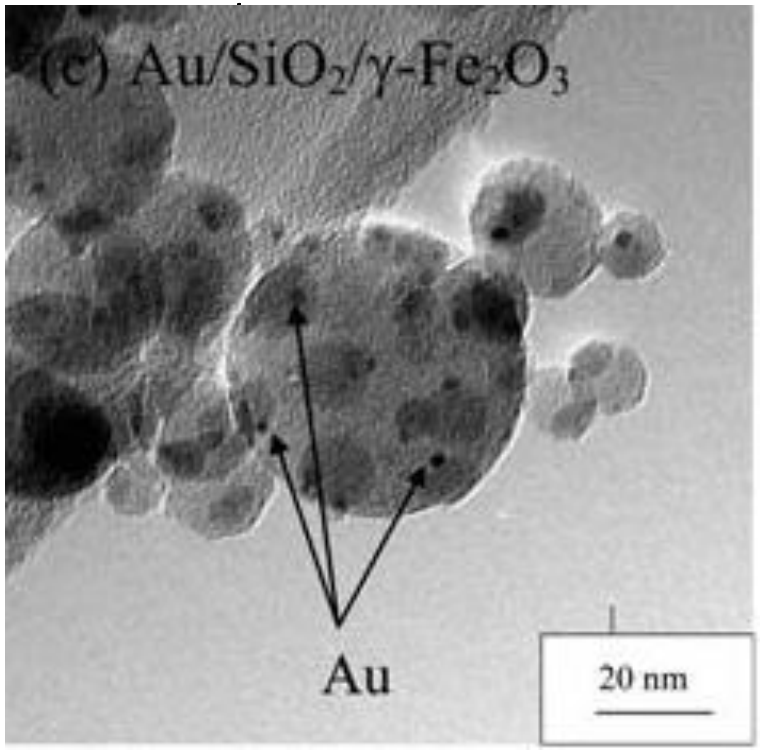
Wey Yang Teoh,a Rose Amala and Lutz M€adler*b
Nanoscale, 2010, 2, 1324–1347



Pd/La$_2$O$_3$/Al$_2$O$_3$
PT-Rh-Ru/Al$_2$O$_3$
Si coated Al-TiO$_2$
Pt-Pd/Al$_2$O$_3$

Y$_3$Al$_5$O$_{12}$
Alpha Al$_2$O$_3$
SiO$_2$, SiO$_2$/ZnO
Ni:MgO-SiO$_2$
Mg$_2$SiO$_4$:Cr
SiO$_2$, SiO$_2$/ZnO$_2$

S. Hannemann, J.-D. Grunwaldt, F. Krumeich,
P. Kappe A. Baiker, Appl. Surf. Sci., 2006, 252, 7862.



Mn$_2$O$_3$
FePO$_4$
Fe$_2$O$_3$
Fe-TiO$_2$
Au-Ag Fe$_2$O$_3$ …

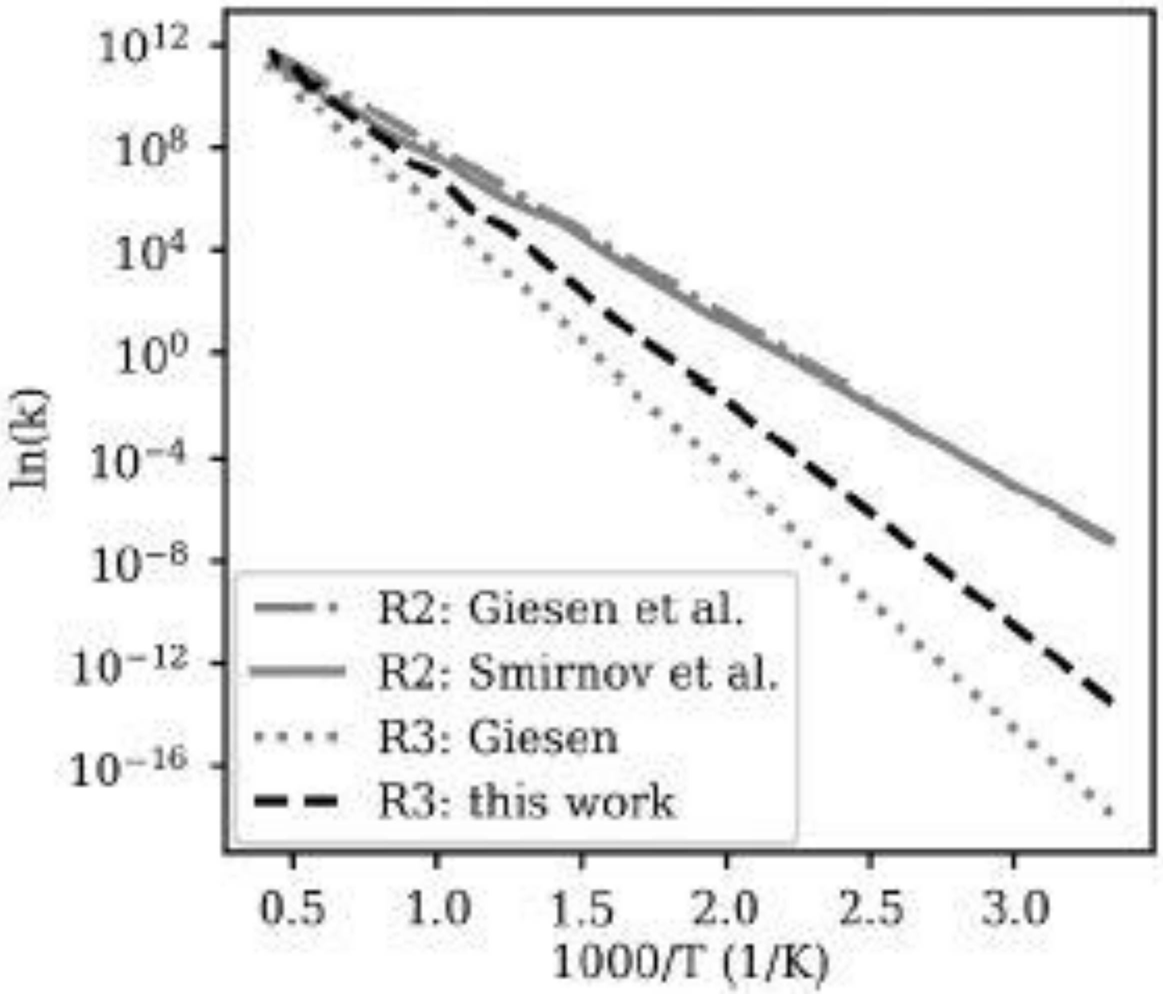

ln(k)
10^{12}
10^{8}
10^{4}
10^{0}
10^{-4}
10^{-8}
10^{-12}
10^{-16}
0.5
1.0
1.5
2.0
2.5
3.0
1000/T (1/K)
R2: Giesen et al.
R2: Smirnov et al.
R3: Giesen
R3: this work

Table II The Reduced Mechanism for Iron Species from $Fe(CO)_5$ in a Flame

No.	Reaction	A	n	E_a	Reference
1	$Fe(CO)_5 \rightarrow Fe + 5CO$	1.93e9	0	72.8	[13]
2	$Fe + O_2 = FeO + O$	1.26e14	0	83.6	[31]
3	$Fe + O_2 + M = FeO_2 + M$	1.50e18	0	83.6	[32]
4	$FeO + H_2O = Fe(OH)_2$	1.63e13	0	0	[24]
5	$FeO + H = Fe + OH$	1.0e14	0	25.08	*E*
6	$FeO + H_2 = Fe + H_2O$	1.0e13	0	20.09	[33]
7	$FeO_2 + OH = FeOH + O_2$	1.0e13	0	50.16	*E*
8	$FeO_2 + O = FeO + O_2$	1.5e14	0	6.27	*E*
9	$FeOH + O = FeO + OH$	5.0e13	0	6.27	*E*
10	$FeOH + H = Fe + H_2O$	1.2e12	0	5.02	*E*
11	$FeOH + H = FeO + H_2$	1.5e14	0	6.69	[24]
12	$Fe(OH)_2 + H = FeOH + H_2O$	2.0e14	0	2.51	[24]
13	$2Fe(OH)_2 = Fe_2O(OH)_2 + H_2O$	8.5e12	0	0	W
14	$Fe_2O(OH)_2 = Fe_2OOOH + H$	1.0e5	0	0	W
15	$Fe_2OOOH + OH \rightarrow Fe_2O_3 + H_2O$	3.0e12	0	0	W
16	$H + O_2 = O + OH$	3.55e15	-0.406	69.39	[17]
17	$O + H_2 = H + OH$	5.08e4	2.67	26.29	[17]
18	$H_2 + OH = H_2O + H$	2.16e8	1.51	14.34	[17]
19	$O + H_2O = OH + OH$	2.97e6	2.02	56.01	[17]
20	$H + OH + M = H_2O + M$	3.8e22	-2	0	[17]
21	$H + O_2 + M = HO_2 + M$	6.37e20	-1.72	2.2	[17]
22	$HO_2 + H = OH + OH$	7.08e13	0	1.233	[17]
23	$HO_2 + O = O_2 + OH$	3.25e13	0	0	[17]
24	$HO_2 + OH = H_2O + O_2$	2.89e13	0	-2.08	[17]
25	$HO_2 + HO_2 = H_2O_2 + O_2$	1.3e11	0	-6.81	[17]
26	$H_2O_2 + M = OH + OH + M$	1.2e17	0	190.2	[17]
27	$CO + OH = CO_2 + H$	2.23e5	1.89	-4.85	[17]

Units of $k_f = A\,T^n \exp(-E_a/RT)$ are cm, s, mol, and kJ, estimated in [4]: *E*, estimations in this work: W. $H_2/O_2/CO$ reactions are taken from the mechanism by Li et al. [17]; for third body efficiencies for reactions (20), (21), and (26), we refer to the cited paper.