

Supplementary Information

Robust Model Developed by LCWR Combined with Uniform Design for the Determination of Hydrogen Peroxide in Water used in micro-gravity environment

Hai-Sheng Dong ^{a,b,*}, Wei Zhao ^b, Ping Cao ^b, Shu-Juan Li ^c, Tong-Fang Liu ^c, Jin-Ming Lin ^a

^a Department of Chemistry, Beijing Key Laboratory of Microanalytical Methods and Instrumentation, MOE Laboratory of Bioorganic Phosphorus Chemistry & Chemical Biology, Tsinghua University, Beijing 100084, China.

^b State Key Lab of Space Medicine Fundamentals and Application, Key Laboratory of Space Nutrition and Food Engineering, China Astronaut Research and Training Center, Beijing, 100094, China.

^c Space Science and Technology Institute (Shenzhen), Shenzhen, 518000, China.

*Corresponding author: Tel/ Fax: +86-010-62792343, E-mail: donghs16@mails.tsinghua.edu.cn (H.-S. Dong)

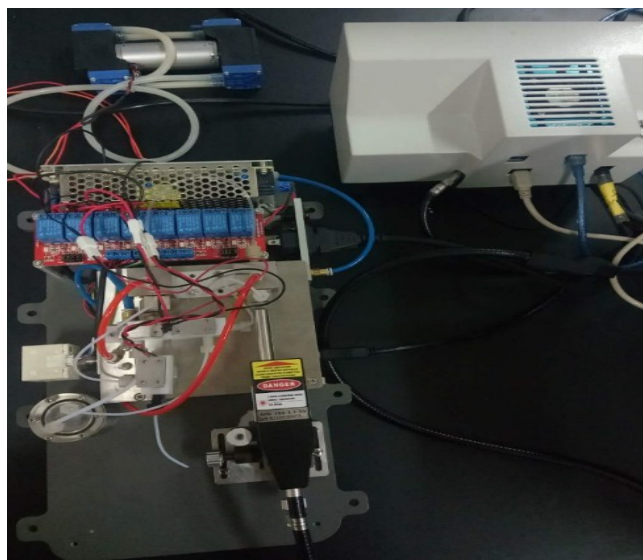


Figure S1 The finally developed testing apparatus: liquid core waveguide Raman spectroscopy

Table S1 Level assignment of concentration for U (6,2) Uniform design

	Concentration(%)	
Level	Sodium nitrate(internal standard)	Hydrogen peroxide
1	1	1.25
2	2	2.5
3	4	5
4	6	7.5
5	8	10
6	10	12.5

Table S2 Concentration distribution of validation set assigned by U (4,2) Uniform design

Samples	Level (concentration %)	
	Hydrogen peroxide	Sodium nitrate
1	4(9)	4(12)
2	2(3)	1(1.5)
3	3(5)	2(3)
4	1(1.5)	2(3)
5	3(5)	3(6)
6	4(9)	1(1.5)
7	1(1.5)	3(6)
8	2(3)	4(12)

Table S3 Samples in calibration set generated by U (6,2) Uniform design

Samples No.	Sodium nitrate (%)	Hydrogen peroxide (%)	Samples No.	Sodium nitrate (%)	Hydrogen peroxide (%)
1	1.25	2	19	7.50	8
2	10.00	8	20	5.00	6
3	7.50	4	21	5.00	1
4	12.50	1	22	7.50	10
5	2.50	2	23	7.50	1
6	1.25	10	24	2.50	4
7	12.50	4	25	1.25	8
8	2.50	1	26	1.25	6
9	2.50	10	27	10.00	4
10	1.25	1	28	5.00	4
11	7.50	2	29	10.00	2
12	10.00	6	30	12.50	10
13	5.00	2	31	12.50	6
14	10.00	10	32	2.50	6
15	12.50	8	33	5.00	8
16	12.50	2	34	7.50	6
17	10.00	1	35	5.00	10
18	2.50	8	36	1.25	4

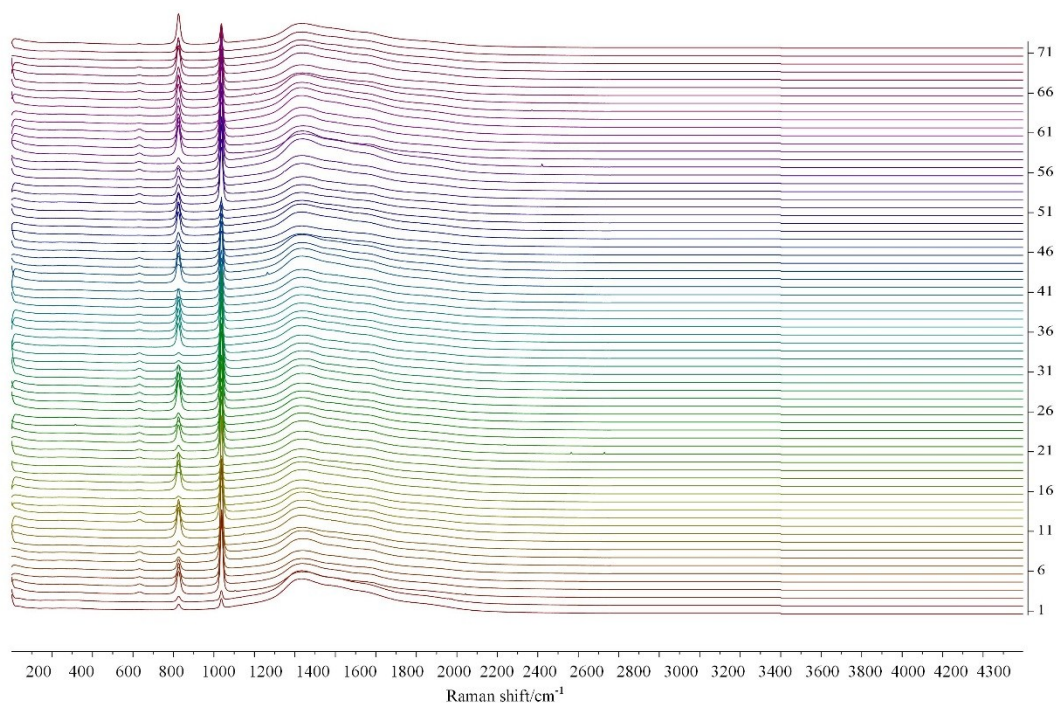


Figure S2 Raman spectra of samples in calibration set obtained by the LCWR apparatus