

Supplementary Information

Figures

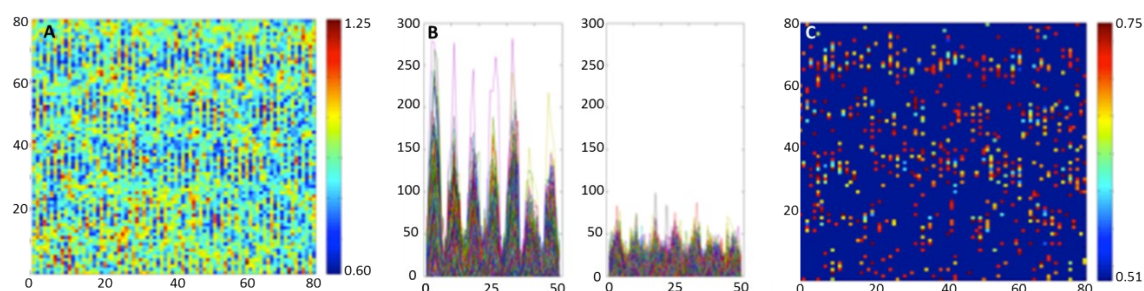


Figure S1 Displayed are the maps and plots representative of signal and noise discrimination of R6G on Klarite 4. (A) Shows a map representative of the MS calculated for the 7 R6G peaks on each of the 6400 spectra taken. (B) The plots demonstrate the discrimination of R6G spectra from noise using a MS value of ≥ 0.75 (R6G signal, left) and ≤ 0.75 (noise, right). (C) The map highlights the areas from which the noise is located.

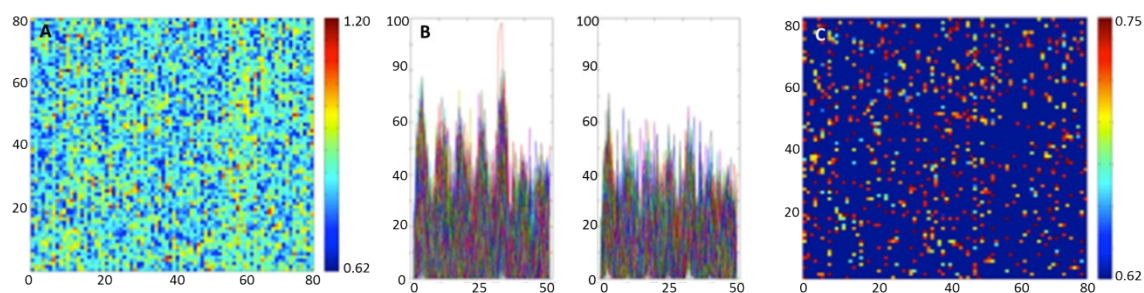


Figure S2 Displayed are the maps and plots representative of signal and noise discrimination of R6G on QSERS 4. (A) Shows a map representative of the MS calculated for the 7 R6G peaks on each of the 6400 spectra taken. (B) The plots demonstrate the discrimination of R6G spectra from noise using a MS value of ≥ 0.75 (R6G signal, left) and ≤ 0.75 (noise, right). (C) The map highlights the areas from which the noise is located.

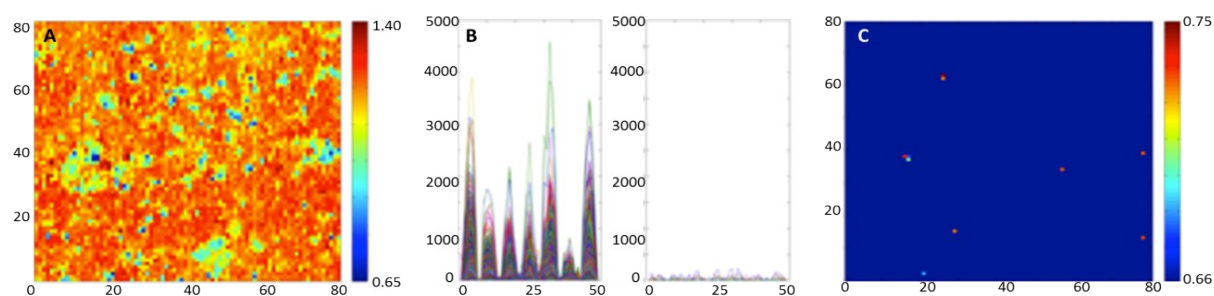


Figure S3 Displayed are the maps and plots representative of signal and noise discrimination of R6G on SoC 5. (A) Shows a map representative of the MS calculated for the 7 R6G peaks on each of the 6400 spectra taken. (B) The plots demonstrate the discrimination of R6G spectra from noise using a MS value of ≥ 0.75 (R6G signal, left) and ≤ 0.75 (noise, right). (C) The map highlights the areas from which the noise is located.

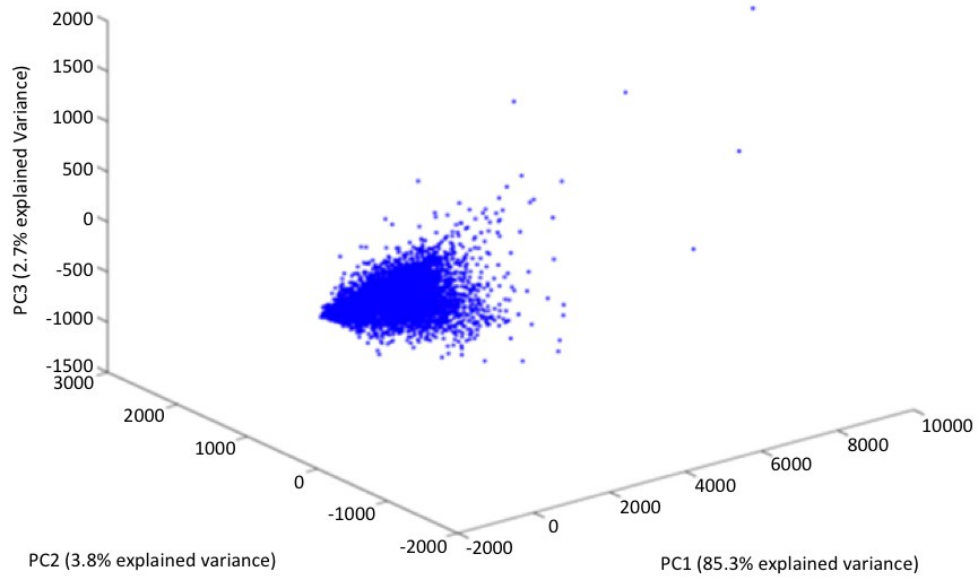


Figure S4 An example PCA plot calculated for SoC 5.

Table S1a Mean peak areas (trapezoidal and sum integration), mean intensities and mean RSDs calculated for Klarite 1.

Klarite 1	Peak Area (Trapezoidal Integration)			Peak Area (Sum Integration)			Intensity			Mean RSDs		
	Peak Number	Mean	SD	RSD	Mean	SD	RSD	Mean	SD	RSD	Peak Area (Trapz)	Peak Area (Sum)
1	165.4	105.3	63.7	166.5	104.8	63	40.1	28.2	70.4	61.7	60.5	74.2
2	117	71.4	61	119.2	70.9	59.5	27.2	20.6	75.8			
3	153.1	94	61.4	154.1	93.5	60.7	43.4	29.6	68.2			
4	104.4	63	60.3	107.7	62.7	58.2	24.2	18.5	76.5			
5	216.2	140	64.7	216.5	139.6	64.5	50.1	34.7	69.3			
6	72.2	38.8	53.7	76.6	39.5	51.6	15.9	13.2	83.1			
7	140.4	94.2	67.1	141.3	93.6	66.3	29.5	22.5	76.3			

Table S1b Mean peak areas (trapezoidal and sum integration), mean intensities and mean RSDs calculated for Klarite 2.

Klarite 2	Peak Area (Trapezoidal Integration)			Peak Area (Sum Integration)			Intensity			Mean RSDs		
	Peak Number	Mean	SD	RSD	Mean	SD	RSD	Mean	SD	RSD	Peak Area (Trapz)	Peak Area (Sum)
1	156.0	91.4	58.6	159.4	91.7	57.5	30.9	22.0	71.3	57.9	56.4	73.8
2	132.8	73.6	55.4	135.3	72.7	53.7	32.5	21.7	66.7			
3	155.3	89.1	57.4	157.3	88.4	56.2	41.0	28.1	68.7			
4	134.3	77.3	57.5	137.6	76.9	55.9	20.7	17.8	85.8			
5	210.3	130.1	61.9	211.3	129.4	61.2	51.0	34.8	68.2			
6	98.8	55.8	56.5	103.3	56.0	54.2	22.1	18.0	81.5			
7	112.8	65.6	58.2	116.2	65.3	56.2	27.8	20.6	74.2			

Table S1c Mean peak areas (trapezoidal and sum integration), mean intensities and mean RSDs calculated for Klarite 3.

Klarite 3	Peak Area (Trapezoidal Integration)			Peak Area (Sum Integration)			Intensity			Mean RSDs		
	Peak Number	Mean	SD	RSD	Mean	SD	RSD	Mean	SD	RSD	Peak Area (Trapz)	Peak Area (Sum)
1	105	56.8	54	109.6	58.2	53.1	17	13.5	79.8	54.6	53.4	71.5
2	102.9	54	52.5	105.2	53.8	51.2	23.2	15.9	68.3			
3	110.5	61.6	55.7	112.4	61.1	54.3	27.9	19.1	68.5			
4	108.2	60.2	55.7	110.4	59.7	54.1	20.2	15.1	75.1			
5	176.7	100.4	56.8	177.3	99.9	56.4	40.1	25.7	64.1			
6	72.9	36.2	49.6	77.1	36.9	47.8	16.4	12.6	77			
7	131.1	76	58	132.2	75.6	57.2	28.3	19.1	67.4			

Table S1d Mean peak areas (trapezoidal and sum integration), mean intensities and mean RSDs calculated for Klarite 4

Klarite 4	Peak Area (Trapezoidal Integration)			Peak Area (Sum Integration)			Intensity			Mean RSDs		
	Peak Number	Mean	SD	RSD	Mean	SD	RSD	Mean	SD	RSD	Peak Area (Trapz)	Peak Area (Sum)
1	144.4	87.3	60.4	146.2	86.6	59.2	32.9	23.2	70.7	56.7	55.2	72.8
2	110.3	62.4	56.6	112.8	61.8	54.8	23.2	17.2	74			
3	106.1	59.1	55.7	109.5	58.5	53.5	23	17.2	75			
4	120.6	65	53.9	123.2	64.9	52.6	23.7	16.7	70.8			
5	149.5	89.7	60	151.3	89	58.9	28	20.7	73.9			
6	86.8	45.2	52.1	89.3	44.9	50.3	21.4	15	70.3			
7	105.9	61.7	58.3	107.6	61.2	56.8	22.7	17.1	75.1			

Table S1e Mean peak areas (trapezoidal and sum integration), mean intensities and mean RSDs calculated for Klarite 5

Klarite 5	Peak Area (Trapezoidal Integration)			Peak Area (Sum Integration)			Intensity			Mean RSDs		
	Peak Number	Mean	SD	RSD	Mean	SD	RSD	Mean	SD	RSD	Peak Area (Trapz)	Peak Area (Sum)
1	185.1	110.4	59.7	186.8	110.4	59.1	41.8	28.3	67.6	58.2	56.8	73.1
2	131.1	76.2	58.1	133.3	75.4	56.6	27.5	21	76.2			
3	122	71.5	58.6	125.5	70.8	56.4	27.7	20.1	72.6			
4	139.3	77.7	55.8	141.6	77.2	54.5	28.6	20.1	70.2			
5	181.9	113.6	62.4	183.5	112.8	61.5	31.9	23.8	74.8			
6	94.6	50.6	53.5	97.1	50	51.5	18.6	14.6	78.4			
7	127.7	75.6	59.3	129	75	58.1	29.6	21.3	71.7			

Table S2a Mean peak areas (trapezoidal and sum integration), mean intensities and mean RSDs calculated for QSERS 1

QSERS 1	Peak Area (Trapezoidal Integration)			Peak Area (Sum Integration)			Intensity			Mean RSDs		
	Peak Number	Mean	SD	RSD	Mean	SD	RSD	Mean	SD	RSD	Peak Area (Trapz)	Peak Area (Sum)
1	202.5	46.8	23.1	202.6	46.6	23	48.4	13.5	27.9	33.7	32.9	59.6
2	98.7	34.4	34.8	100.3	34.1	34	18.8	11.3	59.9			
3	72.8	30.5	41.9	77.3	30.5	39.5	14.6	10.3	70.2			
4	90.2	31.8	35.3	93.1	31.9	34.3	16.1	10.6	65.9			
5	179.6	49.5	27.6	180	49.3	27.4	38.2	13.8	36.2			
6	55.8	21.1	37.8	61.8	23	37.3	7.5	7.6	101.8			
7	79.9	28.6	35.7	81.3	28.3	34.8	17.7	9.8	55.4			

Table S2b Mean peak areas (trapezoidal and sum integration), mean intensities and mean RSDs calculated for QSERS 2

QSERS 2	Peak Area (Trapezoidal Integration)			Peak Area (Sum Integration)			Intensity			Mean RSDs		
	Peak Number	Mean	SD	RSD	Mean	SD	RSD	Mean	SD	RSD	Peak Area (Trapz)	Peak Area (Sum)
1	170.4	40.2	23.6	170.4	40.2	23.6	39.9	11.9	29.8	33	33	51.5
2	95.6	32.4	33.9	95.6	32.4	33.9	23.5	10.9	46.1			
3	69.1	28.2	40.8	69.1	28.2	40.8	15	9.9	66.1			
4	92.9	32.3	34.8	92.9	32.3	34.8	22.9	11.4	49.5			
5	179.7	45.8	25.5	179.7	45.8	25.5	39.8	13.6	34.1			
6	54.6	20.7	37.9	54.6	20.7	37.9	9.3	7.9	84.3			
7	84.4	28.9	34.2	84.4	28.9	34.2	19.7	9.9	50.4			

Table S2c Mean peak areas (trapezoidal and sum integration), mean intensities and mean RSDs calculated for QSERS 3

QSERS 3	Peak Area (Trapezoidal Integration)			Peak Area (Sum Integration)			Intensity			Mean RSDs		
	Peak Number	Mean	SD	RSD	Mean	SD	RSD	Mean	SD	RSD	Peak Area (Trapz)	Peak Area (Sum)
1	117.1	34.2	29.2	118.3	34.1	28.8	29.4	11.8	40.2	34.8	34	63
2	83	28.4	34.2	84.9	28.1	33.1	14.7	9.7	66.3			
3	59.4	23.9	40.2	63.7	24.8	38.9	11.5	9	77.9			
4	80.9	28.2	34.9	83	28	33.8	20.1	10.1	50.3			
5	127.9	37.5	29.3	128.8	37.2	28.9	26.9	12.5	46.4			
6	50.3	18.9	37.5	58	21.5	37.1	8.3	7.6	91.5			
7	63.1	24.4	38.6	65	24.2	37.2	12.7	8.7	68.2			

Table S2d Mean peak areas (trapezoidal and sum integration), mean intensities and mean RSDs calculated for QSERS 4

QSERS 4	Peak Area (Trapezoidal Integration)			Peak Area (Sum Integration)			Intensity			Mean RSDs		
	Peak Number	Mean	SD	RSD	Mean	SD	RSD	Mean	SD	RSD	Peak Area (Trapz)	Peak Area (Sum)
1	103.4	33.4	32.3	103.4	33.4	32.3	25	11.7	47	35.8	35.8	63.9
2	76.3	29.2	38.3	76.3	29.2	38.3	15	10.7	70.8			
3	77.5	27.6	35.7	77.5	27.6	35.7	21.4	11	51.4			
4	76.3	27.2	35.6	76.3	27.2	35.6	15.2	10.3	67.6			
5	112.4	35.6	31.7	112.4	35.6	31.7	25.4	12	47.2			
6	55.9	21.2	37.9	55.9	21.2	37.9	8.5	8	94.1			
7	55.4	21.6	39	55.4	21.6	39	12.6	8.7	69			

Table S2e Mean peak areas (trapezoidal and sum integration), mean intensities and mean RSDs calculated for QSERS 5

QSERS 5	Peak Area (Trapezoidal Integration)			Peak Area (Sum Integration)			Intensity			Mean RSDs		
	Peak Number	Mean	SD	RSD	Mean	SD	RSD	Mean	SD	RSD	Peak Area (Trapz)	Peak Area (Sum)
1	99.8	44.6	44.7	101.1	44.4	43.9	24.4	14.4	58.9	41.1	39.9	66.4
2	69.2	27.5	39.7	72.6	27.8	38.3	14	9.8	70			
3	70.2	26.5	37.8	74.7	27.5	36.8	20.5	13.8	67.2			
4	72.2	29.8	41.3	75.6	30.1	39.8	16.3	10.3	63			
5	113.9	45.8	40.2	115.5	45.6	39.5	26.7	13.6	51			
6	54.8	21.1	38.4	60.2	22.7	37.7	8.8	7.7	87.3			
7	54.1	24.6	45.5	57.8	25.2	43.5	13.2	8.9	67.5			

Table S3a Mean peak areas (trapezoidal and sum integration), mean intensities and mean RSDs calculated for SoC 1

SoC 1	Peak Area (Trapezoidal Integration)			Peak Area (Sum Integration)			Intensity			Mean RSDs		
	Peak Number	Mean	SD	RSD	Mean	SD	RSD	Mean	SD	RSD	Peak Area (Trapz)	Peak Area (Sum)
1	1353.9	739.8	54.6	1362.1	737	54.1	343.7	180.2	52.4	48.6	48.5	54.5
2	1206.2	537.8	44.6	1205.6	537.5	44.6	281.7	126.5	44.9			
3	919.3	425.5	46.3	922.9	426.5	46.2	266.7	121.8	45.7			
4	1161.1	548.3	47.2	1160.8	547.8	47.2	238.4	121.5	51			
5	1217.4	610.7	50.2	1218.5	609.5	50	251.7	134.6	53.5			
6	353	186.6	52.9	406.5	215.6	53	54.3	47.9	88.1			
7	2096.3	930.6	44.4	2095.5	930.4	44.4	502.2	230.1	45.8			

Table S3b Mean peak areas (trapezoidal and sum integration), mean intensities and mean RSDs calculated for SoC 2

SoC 2	Peak Area (Trapezoidal Integration)			Peak Area (Sum Integration)			Intensity			Mean RSDs		
	Peak Number	Mean	SD	RSD	Mean	SD	RSD	Mean	SD	RSD	Peak Area (Trapz)	Peak Area (Sum)
1	1507.5	821.4	54.5	1509.8	819.8	54.3	349.1	185.6	53.2	47.6	47.6	53
2	1015.3	462.5	45.6	1014.9	462.1	45.5	281.9	129.9	46.1			
3	1174.6	529.3	45.1	1174.7	529.1	45	319.9	146.1	45.7			
4	1033.7	484.6	46.9	1034.9	483.7	46.7	227.1	113.3	49.9			
5	2056	941.9	45.8	2055	941.3	45.8	463	223.3	48.2			
6	287.1	145.1	50.5	336.4	170.5	50.7	50.8	41.3	81.2			
7	2417.1	1091.1	45.1	2415.9	1090.6	45.1	587.7	275.3	46.8			

Table S3c Mean peak areas (trapezoidal and sum integration), mean intensities and mean RSDs calculated for SoC 3

SoC 3	Peak Area (Trapezoidal Integration)			Peak Area (Sum Integration)			Intensity			Mean RSDs		
	Peak Number	Mean	SD	RSD	Mean	SD	RSD	Mean	SD	RSD	Peak Area (Trapz)	Peak Area (Sum)
1	1329.1	782.2	58.9	1330	780	58.6	238.3	155.2	65.1	49.8	49.5	55.9
2	1039.7	479.3	46.1	1039.2	479	46.1	228.9	110.8	48.4			
3	1185.6	553.7	46.7	1185.3	553.2	46.7	307.3	144.6	47.1			
4	882.8	448.2	50.8	883.6	447.1	50.6	216.9	115.6	53.3			
5	1786.6	909.2	50.9	1787.7	907.3	50.8	340.5	186.3	54.7			
6	283.1	143.8	50.8	307.4	150.6	49	58.4	44.7	76.5			
7	2747	1221	44.4	2745.6	1220.3	44.4	606.7	279.1	46			

Table S3d Mean peak areas (trapezoidal and sum integration), mean intensities and mean RSDs calculated for SoC 4

SoC 4	Peak Area (Trapezoidal Integration)			Peak Area (Sum Integration)			Intensity			Mean RSDs		
	Peak Number	Mean	SD	RSD	Mean	SD	RSD	Mean	SD	RSD	Peak Area (Trapz)	Peak Area (Sum)
1	1750.3	862.5	49.3	1749.7	861.7	49.3	309.7	162.7	52.5	47.8	47.8	51.7
2	970.4	447	46.1	970.2	446.5	46	212	102.2	48.2			
3	1173.2	537.3	45.8	1172.8	536.8	45.8	324.9	155.9	48			
4	957.1	464.4	48.5	958.8	463.8	48.4	217.8	112.7	51.7			
5	1708.2	846.5	49.6	1707.8	845.6	49.5	343.9	190.2	55.3			
6	500.1	248.6	49.7	526.2	263.7	50.1	113.7	65.5	57.6			
7	1887.7	858.2	45.5	1886.8	857.8	45.5	354.1	172.1	48.6			

Table S3e Mean peak areas (trapezoidal and sum integration), mean intensities and mean RSDs calculated for SoC 5

SoC 5	Peak Area (Trapezoidal Integration)			Peak Area (Sum Integration)			Intensity			Mean RSDs		
	Mean	SD	RSD	Mean	SD	RSD	Mean	SD	RSD	Peak Area (Trapz)	Peak Area (Sum)	Intensity
1	1752	916.2	52.3	1751.3	915.6	52.3	325.4	180.1	55.4	49.3	49.3	53.1
2	1163.1	542.8	46.7	1162.6	542.3	46.6	279.7	134.4	48.1			
3	1028.2	504.6	49.1	1028.4	503.7	49	278.2	148.1	53.2			
4	882.7	446.6	50.6	884.2	445.3	50.4	232.5	121.6	52.3			
5	1933.1	967.5	50.1	1933.3	965.7	50	313	187	59.7			
6	482.9	235.7	48.8	493.7	241.4	48.9	118.4	64.6	54.6			
7	2179.4	1038.7	47.7	2178.3	1038.1	47.7	515.1	248.1	48.2			

Table S4 The seven common R6G peaks used for analysis are shown together with their tentative vibrational assignments. Minima and maxima defined by Raman shift and data point values are also provided.

Peak Number	Raman Shift (cm ⁻¹)			Data Points			Vibrational Assignment
	Peak Start (Minima)	Peak End (Minima)	Maxima	Peak Start (Minima)	Peak End (Minima)	Maxima	
1	602.	621	611	148	154	151	Xanthene Ring Deformation C-C-C ip Bend
2	762	780	771	200	206	203	C-H Out of Plane Bend
3	1173	1190	1182	340	346	343	Unassigned
4	1306	1323	1315	387	393	390	C-C str + C-N Stretch
5	1354	1370	1362	404	410	407	C-C str + C-N Stretch
6	1564	1580	1572	481	487	484	Aromatic C-C Stretch
7	1639	1655	1647	509	515	512	Aromatic C-C Stretch