Wavenumber Standards for Raman Spectrometry

Michael M. Carrabba
Chromex, Inc., Albuquerque, NM, USA

1 INTRODUCTION

Instrument calibration is an important part of Raman analysis. For modern-day applications such as forensic science, the calibration of the Raman instrument needs to be conducted on a daily or even an hourly basis. Raman instruments have been routinely calibrated with the emission lines from low-pressure discharge lamps such as mercury, argon and neon. This technique is fairly well established and used in research-type environments. However, the ability consistently and easily to align atomic-based sources with an instrument is a major disadvantage of this technique. Thus, an unskilled user may induce calibration errors from misalignment. Another problem with modern-day instruments is the actual laser sources used for excitation. Many commercially available Raman spectrometers now use sources that are not based on ion lasers. In the past, these ion-based lasers had excitation frequencies that were well established and stable. However, new laser sources such as diode lasers and tunable (dye and solid-state) lasers do not have established frequencies. With unstable or changeable excitation frequency sources it is more suitable to use samples of known relative wavenumber shift for calibration. This article describes the use of wavenumber shift standards for the calibration of Raman instruments and how the standards were established.

2 STANDARD DEVELOPMENT

The American Society for Testing and Materials (ASTM) Committee on Molecular Spectroscopy invoked on the development of Raman shift standards so that calibrations of a Raman instrument could be accomplished when the frequency of the excitation source was unknown.[1] Many studies have discussed the methodology of the calibration procedure including the use of atomic-based light sources.[2–7] These procedures will not be discussed in this article, however, as for highly stable laser frequency sources such as argon ion, krypton ion and He–Ne this methodology works fairly well. For reference purposes, Tables 1 and 2 contain the absolute wavenumber positions and the Raman shift positions for neon and argon atomic lines.[8] The Raman shift positions are shown for 488.0-, 514.5-, 632.8- and 647.1-nm excitation.

For Raman shift standards, a variety of materials needed to be chosen that would both cover a range of solids and liquids and have numerous Raman bands for calibration in the region of 85–3300 cm^{-1}. Eight materials (Table 3) were selected that were readily available from commercial sources at high purity. For the ASTM study, the materials were sent out for examination on different instruments [Fourier transform (FT), scanning dispersive and multichannel] at several laboratories. The laboratories were not provided detailed calibration information, only spectra that contained no peak frequencies. The calibration method for each instrument was left up to the individual laboratories. The detailed results can be found in the ASTM Standard Guide for the study.[1]

Table 3 summarizes the results and presents certain data from a subsequent study by Mann *et al*., who examined several of the samples with high precision and accuracy.[6,7] To provide a guide for relative intensities, spectra of several of the standard materials obtained with a diode laser that was operating in the region of 785 nm are presented in Figure 1. Note that the absolute laser frequency was unknown and the instrument was calibrated against the Raman shifts established in the ASTM Standard Guide. The spectra presented have been corrected for instrument response.

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Table 1. Neon calibration lines.

Neon lines[8]		Calculated Raman shift (cm^{-1})				
Wavelength (nm)	Wavenumber (cm^{-1})	488.0 nm	514.5 nm	632.8 nm	647.1 nm	785.0 nm
475.2732	21040.53	−548.73	−1604.18			
478.8927	20881.50	−389.70	−1445.16			
479.0220	20875.87	−384.06	−1439.52			
482.7344	20715.33	−223.52	−1278.98			
488.4917	20471.18	20.63	−1034.83			
500.5159	19979.39	512.42	−543.04	−4176.60		
503.7751	19850.13	641.68	−413.78	−4047.35	−4396.57	
514.4938	19436.58	1055.22	−0.23	−3633.80	−3983.02	
533.0778	18758.99	1732.82	677.36	−2956.21	−3305.43	
534.1094	18722.76	1769.05	713.59	−2919.97	−3269.19	
534.3283	18715.09	1776.72	721.26	−2912.30	−3261.52	
540.0562	18516.59	1975.21	919.75	−2713.81	−3063.03	
556.2766	17976.67	2515.13	1459.68	−2173.89	−2523.11	
565.6659	17678.28	2813.52	1758.07	−1875.50	−2224.72	
571.9225	17484.89	3006.92	1951.46	−1682.11	−2031.32	
574.8298	17396.45	3095.35	2039.89	−1593.67	−1942.89	
576.4419	17347.80	3144.00	2088.54	−1545.02	−1894.24	
580.4450	17228.16	3263.64	2208.18	−1425.38	−1774.60	
582.0156	17181.67	3310.13	2254.68	−1378.89	−1728.11	
585.2488	17086.75	3405.05	2349.60	−1283.97	−1633.19	
587.2828	17027.57	3464.23	2408.77	−1224.79	−1574.01	−4288.72
588.1895	17001.32	3490.48	2435.02	−1198.54	−1547.76	−4262.47
590.2462	16942.08	3549.72	2494.26	−1139.30	−1488.52	−4203.23
590.6429	16930.70	3561.10	2505.64	−1127.92	−1477.14	−4191.85
594.4834	16821.33	3670.48	2615.02	−1018.55	−1367.77	−4082.47
596.5471	16763.14	3728.67	2673.21	−960.35	−1309.57	−4024.28
597.4627	16737.45	3754.36	2698.90	−934.67	−1283.88	−3998.59
597.5534	16734.91	3756.90	2701.44	−932.12	−1281.34	−3996.05
598.7907	16700.33	3791.48	2736.02	−897.54	−1246.76	−3961.47
602.9997	16583.76	3908.05	2852.59	−780.97	−1130.19	−3844.90
607.4338	16462.70	4029.10	2973.65	−659.92	−1009.14	−3723.85
609.6163	16403.76	4088.04	3032.59	−600.98	−950.20	−3664.91
612.8450	16317.34	4174.46	3119.01	−514.56	−863.78	−3578.49
614.3063	16278.52	4213.28	3157.82	−475.74	−824.96	−3539.67
616.3594	16224.30	4267.50	3212.05	−421.52	−770.74	−3485.45
618.2146	16175.61		3260.73	−372.83	−722.05	−3436.76
621.7281	16084.20		3352.14	−281.42	−630.64	−3345.35
626.6495	15957.88		3478.46	−155.10	−504.32	−3219.03
630.4789	15860.96		3575.39	−58.18	−407.40	−3122.11
632.8165	15802.37		3633.98	0.41	−348.81	−3063.52
633.4428	15786.75		3649.60	16.04	−333.18	−3047.89
638.2992	15666.63		3769.71	136.15	−213.07	−2927.78
640.2246	15619.52		3816.83	183.26	−165.96	−2880.67
650.6528	15369.18		4067.17	433.60	84.38	−2630.33
659.2882	15167.87		4268.47	634.91	285.69	−2429.02
665.2093	15032.86			769.92	420.70	−2294.01
667.8276	14973.92			828.86	479.64	−2235.07
671.7043	14887.50			915.28	566.06	−2148.65
692.9467	14431.12			1371.66	1022.44	−1692.27
702.4050	14236.80			1565.98	1216.76	−1497.95
703.2413	14219.87			1582.91	1233.69	−1481.02
705.1292	14181.80			1620.98	1271.76	−1442.94
705.9107	14166.10			1636.68	1287.46	−1427.24
717.3938	13939.35			1863.44	1514.22	−1200.49

(*continued overleaf*)

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Table 1. (*continued*)

Neon lines[8]		Calculated Raman shift (cm^{-1})				
Wavelength (nm)	Wavenumber (cm^{-1})	488.0 nm	514.5 nm	632.8 nm	647.1 nm	785.0 nm
724.5167	13802.30			2000.48	1651.26	−1063.45
747.2439	13382.51			2420.27	2071.05	−643.66
748.8871	13353.15			2449.63	2100.41	−614.29
753.5774	13270.04			2532.74	2183.53	−531.18
754.4044	13255.49			2547.29	2198.07	−516.64
772.4628	12945.61			2857.17	2507.95	−206.75
783.9055	12756.64			3046.14	2696.92	−17.79
792.7118	12614.93			3187.86	2838.64	123.93
793.6996	12599.23			3203.56	2854.34	139.63
794.3181	12589.41			3213.37	2864.15	149.44
808.2458	12372.47			3430.31	3081.09	366.38
811.8549	12317.47			3485.31	3136.09	421.38
812.8911	12301.77			3501.01	3151.79	437.08
813.6406	12290.44			3512.34	3163.12	448.41
825.9379	12107.45			3695.33	3346.11	631.41
826.6077	12097.64			3705.14	3355.92	641.22
826.7117	12096.12			3706.67	3357.45	642.74
830.0326	12047.72			3755.06	3405.84	691.13
836.5749	11953.50			3849.28	3500.06	785.35
837.7606	11936.58			3866.20	3516.98	802.27
841.7159	11880.49			3922.29	3573.07	858.36
841.8427	11878.70			3924.08	3574.86	860.15
846.3358	11815.64			3987.14	3637.92	923.21
848.4444	11786.28			4016.51	3667.29	952.58
849.5360	11771.13			4031.65	3682.43	967.72
854.4696	11703.17			4099.61	3750.40	1035.69
857.1352	11666.77			4136.01	3786.79	1072.08
859.1259	11639.74			4163.04	3813.82	1099.12
863.4647	11581.25			4221.53	3872.31	1157.60
864.7041	11564.65			4238.13	3888.91	1174.20
865.4383	11554.84			4247.94	3898.72	1184.01
865.5522	11553.32			4249.46	3900.24	1185.54
867.9492	11521.41			4281.37	3932.15	1217.44
868.1921	11518.19			4284.59	3935.37	1220.67
870.4112	11488.82				3964.74	1250.03
877.1656	11400.36				4053.21	1338.50
878.0621	11388.72				4064.85	1350.14
878.3753	11384.66				4068.91	1354.20
883.0907	11323.87				4129.70	1414.99
885.3867	11294.50				4159.06	1444.35
886.5306	11279.93				4173.64	1458.93
886.5755	11279.36				4174.21	1459.50
891.9501	11211.39				4242.17	1527.46
898.8570	11125.24					1613.61
914.8670	10930.55					1808.30
920.1760	10867.49					1871.37
922.0060	10845.92					1892.94
922.1580	10844.13					1894.72
922.6690	10838.12					1900.73
927.5520	10781.07					1957.79
930.0850	10751.71					1987.15
931.0580	10740.47					1998.38
931.3970	10736.56					2002.29
932.6510	10722.12					2016.73
937.3310	10668.59					2070.26

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Table 1. (*continued*)

Neon lines[8]		Calculated Raman shift (cm^{-1})				
Wavelength (nm)	Wavenumber (cm^{-1})	488.0 nm	514.5 nm	632.8 nm	647.1 nm	785.0 nm
942.5380	10609.65					2129.20
945.9210	10571.71					2167.15
948.6680	10541.10					2197.76
953.4160	10488.60					2250.25
954.7400	10474.06					2264.80
966.5420	10346.16					2392.69
1029.542	9713.057					3025.80
1056.241	9467.536					3271.32
1079.807	9260.914					3477.94
1084.348	9222.132					3516.72
1114.302	8974.228					3764.63
1117.753	8946.522					3792.33

Table 2. Argon calibration lines.

Argon line[8]		Calculated Raman shift (cm^{-1})				
Wavelength (nm)	Wavenumber (cm^{-1})	488.0 nm	514.5 nm	632.8 nm	647.1 nm	785.0 nm
515.1391	19412.23	1079.57	24.11	−3609.45	−3958.67	
516.2285	19371.27	1120.54	65.08	−3568.49	−3917.70	
518.7746	19276.19	1215.61	160.15	−3473.41	−3822.63	
522.1271	19152.42	1339.38	283.92	−3349.64	−3698.86	
542.1352	18445.58	2046.22	990.76	−2642.80	−2992.02	
545.1652	18343.06	2148.74	1093.28	−2540.28	−2889.50	
549.5874	18195.47	2296.34	1240.88	−2392.69	−2741.91	
550.6113	18161.63	2330.17	1274.71	−2358.85	−2708.07	
555.8702	17989.81	2501.99	1446.53	−2187.03	−2536.25	
557.2541	17945.13	2546.67	1491.21	−2142.35	−2491.57	
560.6733	17835.70	2656.10	1600.65	−2032.92	−2382.14	
565.0704	17696.91	2794.89	1739.44	−1894.13	−2243.35	
573.9520	17423.06	3068.74	2013.29	−1620.28	−1969.50	
583.4263	17140.13	3351.68	2296.22	−1337.34	−1686.56	
586.0310	17063.94	3427.86	2372.40	−1261.16	−1610.38	
588.2624	16999.22	3492.59	2437.13	−1196.44	−1545.65	
588.8584	16982.01	3509.79	2454.33	−1179.23	−1528.45	
591.2085	16914.51	3577.30	2521.84	−1111.73	−1460.94	
592.8813	16866.78	3625.02	2569.56	−1064.00	−1413.22	
594.2669	16827.46	3664.35	2608.89	−1024.67	−1373.89	
598.7302	16702.01	3789.79	2734.33	−899.23	−1248.45	−3963.16
599.8999	16669.45	3822.36	2766.90	−866.67	−1215.89	−3930.59
602.5150	16597.10	3894.71	2839.25	−794.32	−1143.54	−3858.24
603.2127	16577.90	3913.90	2858.45	−775.12	−1124.34	−3839.05
604.3223	16547.46	3944.34	2888.88	−744.68	−1093.90	−3808.61
605.2723	16521.49	3970.31	2914.86	−718.71	−1067.93	−3782.64
605.9372	16503.36	3988.44	2932.99	−700.58	−1049.80	−3764.51
609.8803	16396.66		3039.69	−593.88	−943.10	−3657.81
610.5635	16378.31		3058.03	−575.53	−924.75	−3639.46
614.5441	16272.23		3164.12	−469.44	−818.66	−3533.37
617.0174	16207.00		3229.35	−404.22	−753.44	−3468.14
617.3096	16199.33		3237.02	−396.55	−745.76	−3460.47
621.2503	16096.57		3339.77	−293.79	−643.01	−3357.72
621.5938	16087.68		3348.67	−284.90	−634.11	−3348.82
629.6872	15880.90		3555.45	−78.12	−427.34	−3142.05
630.7657	15853.75		3582.60	−50.97	−400.19	−3114.89

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Table 2. (*continued*)

Argon line[8]		Calculated Raman shift (cm^{-1})				
Wavelength (nm)	Wavenumber (cm^{-1})	488.0 nm	514.5 nm	632.8 nm	647.1 nm	785.0 nm
636.9575	15699.63		3736.71	103.15	−246.07	−2960.78
638.4717	15662.40		3773.94	140.38	−208.84	−2923.55
641.6307	15585.29		3851.06	217.49	−131.73	−2846.44
653.8112	15294.94			507.85	158.63	−2556.08
660.4853	15140.38			662.40	313.18	−2401.53
666.0676	15013.49			789.29	440.07	−2274.64
666.4051	15005.89			796.89	447.67	−2267.03
667.7282	14976.15			826.63	477.41	−2237.30
675.2834	14808.60			994.18	644.96	−2069.74
675.6163	14801.30			1001.48	652.26	−2062.45
676.6612	14778.44			1024.34	675.12	−2039.59
687.1289	14553.31			1249.47	900.25	−1814.46
687.9582	14535.77			1267.01	917.80	−1796.91
688.8174	14517.64			1285.15	935.93	−1778.78
693.7664	14414.07			1388.71	1039.49	−1675.22
695.1478	14385.43			1417.35	1068.13	−1646.58
696.0250	14367.30			1435.48	1086.26	−1628.45
696.5431	14356.61			1446.17	1096.95	−1617.76
703.0251	14224.24			1578.54	1229.32	−1485.39
706.7218	14149.84			1652.94	1303.72	−1410.99
706.8736	14146.80			1655.98	1306.76	−1407.95
710.7478	14069.69			1733.09	1383.87	−1330.83
712.5820	14033.47			1769.31	1420.09	−1294.62
714.7042	13991.80			1810.98	1461.76	−1252.95
715.8839	13968.75			1834.04	1484.82	−1229.89
720.6980	13875.44			1927.34	1578.12	−1136.58
726.5172	13764.30			2038.48	1689.26	−1025.45
727.0664	13753.90			2048.88	1699.66	−1015.05
727.2936	13749.61			2053.18	1703.96	−1010.75
731.1716	13676.68			2126.10	1776.88	−937.83
731.6005	13668.66			2134.12	1784.90	−929.81
735.0814	13603.94			2198.85	1849.63	−865.08
735.3293	13599.35			2203.43	1854.21	−860.50
737.2118	13564.62			2238.16	1888.94	−825.77
738.3980	13542.83			2259.95	1910.73	−803.98
739.2980	13526.35			2276.44	1927.22	−787.49
741.2337	13491.02			2311.76	1962.54	−752.17
742.5294	13467.48			2335.30	1986.08	−728.63
743.5368	13449.23			2353.55	2004.33	−710.38
743.6297	13447.55			2355.23	2006.01	−708.70
750.3869	13326.46			2476.32	2127.10	−587.61
751.4652	13307.34			2495.45	2146.23	−568.48
763.5106	13097.40			2705.39	2356.17	−358.54
772.3761	12947.06			2855.72	2506.50	−208.21
772.4207	12946.31			2856.47	2507.25	−207.46
789.1075	12672.54			3130.24	2781.02	66.31
794.8176	12581.50			3221.28	2872.06	157.35
800.6157	12490.39			3312.39	2963.17	248.47
801.4786	12476.94			3325.84	2976.62	261.91
805.3308	12417.26			3385.52	3036.30	321.60
810.3693	12340.05			3462.73	3113.51	398.80
811.5311	12322.39			3480.39	3131.18	416.47
826.4522	12099.91			3702.87	3353.65	638.94
839.2270	11915.73			3887.05	3537.83	823.13
840.8210	11893.14			3909.64	3560.42	845.72

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Table 2. (*continued*)

Argon line[8]		Calculated Raman shift (cm^{-1})				
Wavelength (nm)	Wavenumber (cm^{-1})	488.0 nm	514.5 nm	632.8 nm	647.1 nm	785.0 nm
842.4648	11869.93			3932.85	3583.63	868.92
852.1442	11735.10				3718.46	1003.75
860.5776	11620.10				3833.46	1118.75
866.7944	11536.76				3916.80	1202.09
884.9910	11299.55					1439.30
907.5394	11018.81					1720.05
912.2967	10961.35					1777.51
919.4638	10875.90					1862.95
922.4499	10840.70					1898.16
929.1531	10762.49					1976.36
935.4220	10690.36					2048.49
965.7786	10354.34					2384.51
1005.206	9948.21					2790.64
1033.272	9677.99					3060.86
1047.005	9551.05					3187.80
1047.803	9543.78					3195.08

Table 3. Raman shift positions (cm^{-1}): average ± standard deviation.

Vickers and Mann:[7] Cyclohexane	ASTM[1]			
	Cyclohexane	Naphthalene	4-Acetamidophenol	Toluene (T)–acetonitrile (A)
			213.3 ± 1.77	
383.81 ± 0.10	384.1 ± 0.78		329.2 ± 0.52	378.5 ± 0.92 (A)
426.62 ± 0.075	426.3 ± 0.41		390.9 ± 0.76	
			465.1 ± 0.30	
		513.8 ± 0.31	504.0 ± 0.60	521.7 ± 0.34 (T)
			651.6 ± 0.50	
			710.8 ± 0.68	
801.39 ± 0.040	801.3 ± 0.96	763.8 ± 0.31	797.2 ± 0.48	786.5 ± 0.40 (T)
			834.5 ± 0.46	
			857.9 ± 0.50	919.0 ± 0.40 (A)
			968.7 ± 0.60	1003.6 ± 0.37 (T)
1028.13 ± 0.041	1028.3 ± 0.45	1021.6 ± 0.49		1030.6 ± 0.36 (T)
			1105.5 ± 0.27	
1157.64 ± 0.051	1157.6 ± 0.94	1147.2 ± 0.34	1168.5 ± 0.65	
			1236.8 ± 0.46	1211.4 ± 0.32 (T)
1265.91 ± 0.10	1266.4 ± 0.58		1278.5 ± 0.45	
1347.57 ± 0.10			1323.9 ± 0.46	
		1382.2 ± 0.31	1371.5 ± 0.11	
1443.73 ± 0.29	1444.4 ± 0.30	1464.5 ± 0.29	1515.1 ± 0.70	
		1576.6 ± 0.29	1561.5 ± 0.52	
			1648.4 ± 0.50	1605.1 ± 0.47 (T)
				2253.7 ± 0.42 (A)
2633.99 ± 0.047				2292.6 ± 0.89 (A)
2665.34 ± 0.047	2664.4 ± 0.42			
2853.59 ± 0.038	2852.9 ± 0.32			
2924.24 ± 0.032	2923.8 ± 0.36		2931.1 ± 0.63	
2938.84 ± 0.048	2938.3 ± 0.51			2940.8 ± 0.25 (A)
		3056.4 ± 0.41	3064.6 ± 0.31	3057.1 ± 0.63 (T)
			3102.4 ± 0.95	
			3326.6 ± 2.18	

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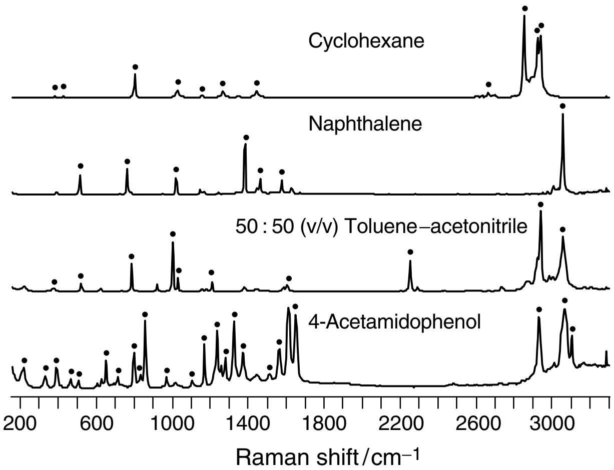

Figure 1. Raman spectra of four ASTM Raman shift standards: cyclohexane, naphthalene, 50 : 50 (v/v) toluene–acetonitrile mixture and 4-acetamidophenol. The spectra have been corrected for instrument response and the Raman bands in Table 3 are indicated on the plots with (●). The spectra were taken at ∼785 nm using a Chromex R2000 instrument operating with a 300 grooves mm^{-1} grating, a 10-μm slit (∼3-cm^{-1} resolution) and integration times of 3–30 s.

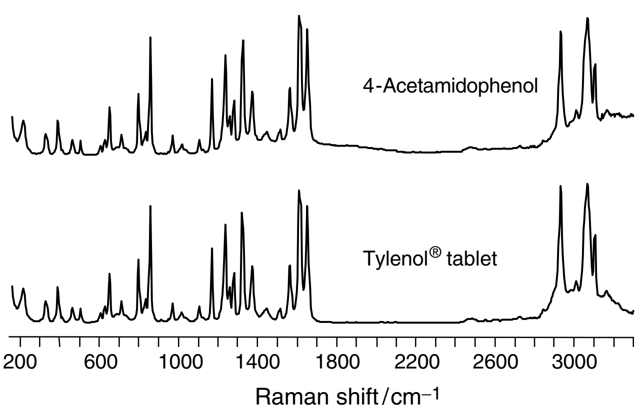

Figure 2. Raman spectra of 4-acetamidophenol and an off-the-shelf Tylenol® tablet. The spectra have been corrected for instrument response and were taken at ∼785 nm using a Chromex R2000 instrument operating with a 300 grooves mm^{-1} grating, a 10-μm slit (∼3-cm^{-1} resolution) and integration times of 30 and 15 s, respectively. Tylenol® is a registered trademark of McNeil-PPC.

With the exception of low-frequency ($<200\,cm^{-1}$) or highly accurate ($\pm 2\,cm^{-1}$) mid-range ($2000–2700\,cm^{-1}$) calibration, most of the standards provide an excellent means of calibration. For general calibration, however, 4-acetamidophenol (acetaminophen, paracetamol) seems to be an excellent choice. This material is the active ingredient in many over-the-counter pain relievers. Acetaminophen is easy to obtain in tablet form and the binding components provide little or no contribution to the spectra. A comparison of a 4-acetamidophenol and a commercial acetaminophen tablet is presented in Figure 2.

3 USE OF SHIFT STANDARDS TO CALIBRATE AN INSTRUMENT

Once Raman data have been acquired from a suitable shift standard, the instrument calibration can be checked. If the observed band positions agree with the reference data to within an acceptable error, the instrument is adequately calibrated. But what if the observed band positions are in error? If each band is offset from its accepted "true" position by the same wavenumber increment, the most likely problem is simply that the laser wavelength in the instrument software is incorrect, giving a constant Raman shift offset across the spectrum. This can be simply corrected by adjusting the laser position (in cm^{-1}) in the software to account for the discrepancy. In this case, the shift standard is being used to measure the laser wavelength. However, if the band position discrepancy is not just a simple offset across the spectrum, it is plausible that the spectrometer is incorrectly calibrated (i.e. the absolute wavelength/wavenumber is not correctly assigned to each spectral element). In this case, one could carry out an absolute calibration using an atomic line source, and then use the shift standard again to measure the laser position. Alternatively, since the Raman shifts of many of the bands in the standard sample are known, these data can be used to perform a least-squares fit relating spectral channel number to actual Raman shift.

4 CONCLUSION

The ASTM Raman shift standard was developed to provide accurate wavenumber shifts from readily available commercial materials. These materials can then be utilized to calibrate any Raman spectrometer, including spectrometers that use variable excitation sources. The use of atomic-based lines can provide a more accurate calibration of a spectrometer; however, the shift standard provides an easy way to calibrate routinely an instrument using the actual collection geometry of the apparatus.

ABBREVIATIONS AND ACRONYMS

ASTM	American Society for Testing and Materials

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