Supporting Information for: Classification of Recycled Plastics using Sparse and Imbalanced Spectral Data and Data Augmentation by the Generative Adversarial Network

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Table S1. Hyperparameters of the GAN framework.

Hyperparameter	**Value**
Epochs	150
Optimizer	Adam
Learning rate (Momentum)	0.0002 ($\beta_1 = 0.5$, $\beta_2 = 0.9$)
Number of Kernels in each block (Discriminator)	Conv2D with (64, 128, 128, 256 channels)
Number of Kernels in each block (Generator)	Conv2D Transpose with (128, 128, 64, channels)
Kernel sizes	(4, 4)
Strides	(2, 2)
Padding	Same
Activation functions	LeakyRelu, Tanh
Kernel initializer	Random normal (sd=0.02)
Slope of Leaky ReLU	0.2

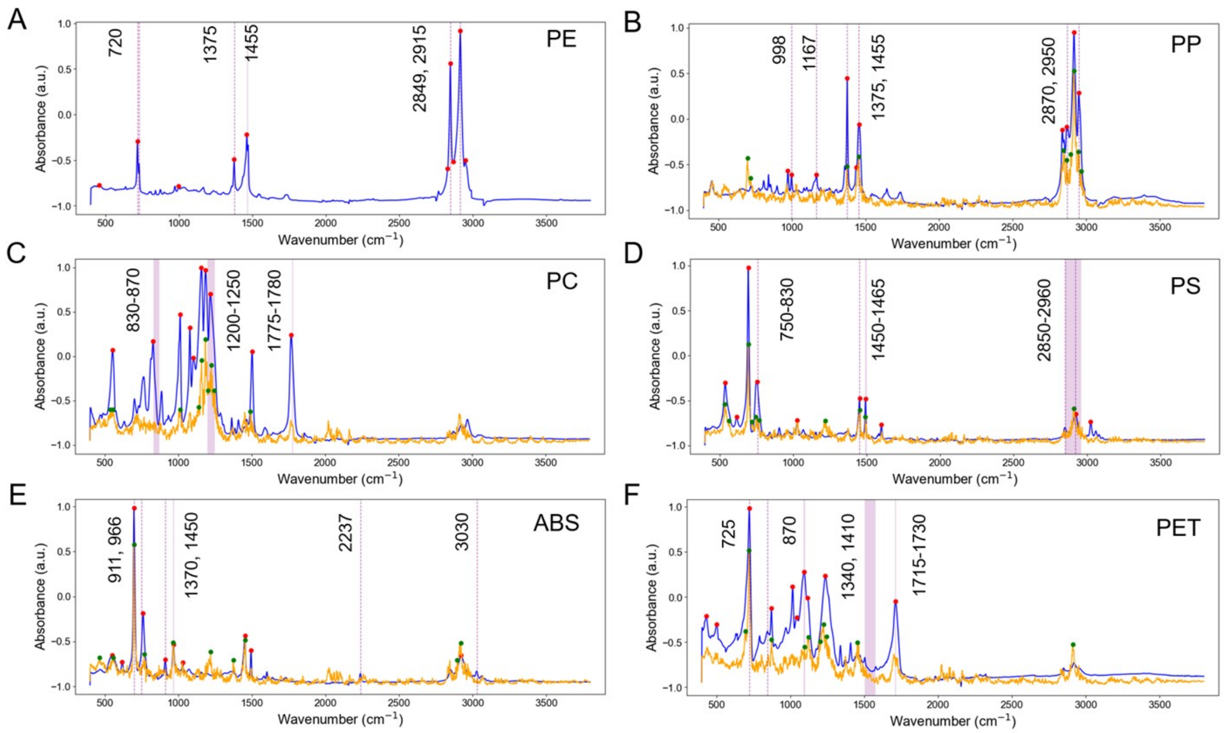

Figure S1. Comparison of GAN-generated synthetic spectral data and real spectral data obtained by replicate experimental measurements on the same samples used to generate Dataset 2. (**A-F**: PE, PP, PC, PS, ABS, and PET, respectively). The blue curves show real (i.e., experimental) FTIR spectra, while the orange curves depict corresponding synthetic spectra generated via GAN. Largest six peaks (i.e., modes) identified from real and synthetic spectra (red and green dots, respectively). As PE is the majority class, no synthetic data were generated.

Table S2. Description of characteristic peaks in the FTIR spectra of PE, PP, PC, PS, ABS, and PET.

Class Label	Polymer	Observed Peaks (cm^{-1})	Characteristic Peaks (cm^{-1})	Functional Group / Assignment
0	PE	1359.82	~1377	CH_3 bending (very weak, likely due to trace branching or chain ends)
		619.15		
		2831.5	2849	CH_2 asymmetric and symmetric stretching
		2935.66	2915	CH_2 asymmetric and symmetric stretching
		715.59	730, 720	CH_2 rocking (crystalline and amorphous)
		1467.83	1465-1472	CH_2 bending and symmetric deformation
1	PP	2825.72	2950, 2870	CH_3 asymmetric and symmetric stretching
		1174.65	1167, 998	C–CH_3 bending and skeletal vibration
		408.91		
		711.73		
		542		
		1365.6	1455, 1375	CH_3 bending and symmetric deformation
2	PC[†]	842.89	830–870	Aromatic C–H bending
		997.2		
		555.5		
		759.95		
		1784.15	1775–1780	C=O stretching (carbonate group)
		1095.57	1200-1250	O–C–O asymmetric stretching
3	PS	2378	2850 – 2960	C-H stretching: CH2, CH3 (backbone)
		1936.53		
		2920.23	2920, 2850	Aliphatic C–H stretching (CH_2 backbone)
		576.72		
		1450.47	1450	CH_2 bending with aromatic ring contribution
			1490-1500	Aromatic C=C stretching (phenyl ring)
		761.88	760, 698-700	Aromatic C–H out-of-plane bending (monosubstituted benzene ring)
4	ABS		2237	C≡N stretching (nitrile, acrylonitrile units)
		2920.23	~3030	Aromatic C–H stretches
		557.43		
		667.37		
		966.34	965-970	Trans-1,4-butadiene =C–H out-of-plane bending
			910	Vinyl =CH_2 out-of-plane wag
		746.45	~750, 700	Aromatic C–H out-of-plane bending (styrene ring)
		1452.4		
5	PET	846.75	845	Methylene (–CH_2–) rocking
		1683.86	1710–1715	C=O stretching (ester group)

		970.19		
		1471.69	1578-1505	In-plane C=C ring
			723	Aromatic C–H out-of-plane bend
		694.37		
		1058.92	1090-1100	C–O stretching vibrations (ester, O–CH_2)

† Weak CH_3 vibrations (~2960–2870 cm^{-1} and ~1360–1380 cm^{-1}) observed in polycarbonate originate from the isopropylidene – $C(CH_3)_2$ – groups of Bisphenol-A units and are not considered primary diagnostic peaks.

Code Availability: The complete code for implementing the GAN framework is available from the corresponding authors upon reasonable request.