

Supplement Material

Classes of compounds taken into account for FTIR absorption bands interpretation are listed in Table S1. A few authentic chemical standards for individual compounds presents each class of compounds because their multifunctional structure. In [1,2] only one absorbance peak was used to quantify a given functional group. However, the peak within a PM spectrum is the collective absorbance of many different molecular bonds that absorb around the same frequency. Therefore, in Table S2 the wavenumber ranges are presented for functionalities found in a few classes of organic and inorganic compounds, according to an approach presented by [3]. [4] database was used as the general guides. Although the standards were used for relatively small number of compounds, FTIR data interpretation performed can assigned all identified absorption peaks to corresponding functionalities of compounds in a given class.

Table S1. Classes and standards of organic and inorganic compounds used for identification of functional groups in ambient aerosols.

Classes	Compounds
alkanes	octacosane;hexadecane;dodecane;hexane
alkenes	hexene
polyaromatics	pyrene;anthracene;benzene;naphthalene
carboxylic acid	benzoic;phtalic;trimellitic;p-nitrobenzoyl glutamic;oxalic;maleic;stearic;adipic ;lauric;p-dimethylaminobenzaldehyde;n-heptanoic;propionic;succinic
carbohydrates	levoglucosan;cellulose
amino acid	p-aminobenzoic acid;cystein;tyrosin;DL-phenylalanine;tryptophan;glycin;valine
amines	diphenylamine;triphenylamine
aldehydes	p-dimethylaminobenzaldehyde;salicyclic aldehydes;p-anisaldehydes;n-butyaldehyde
ketones	acetone;methyl ethyl ketone;methyl isobuthyl ketone;acetylacetone;fluorenone
alcohols	ethanol;methanol;myristic alcohol;sorbitol;antranol;octadecyl alcohol;mannitol
esters	mecopropmethylester;terephthalic acid dimethyl ester;ethyl acetate;sodium acetate;potassium acetate
lactones	4-valerolactone;butyrolactone
quinone	ethanol;methanol;myristic alcohol;sorbitol;antranol;octadecyl alcohol;mannitol
nitrocompounds	p-nitrophenol;2,4 dinitrophenol;2,4 dinitrochlorobenzene;2,4 dinitrophenylhydrazine;m-nitrophenol;p-aminophenol
nitrates	KNO ₃ ;NaNO ₃ ;NH ₄ NO ₃ ;Ca(NO ₃) ₂
carbonates	CaCO ₃ ;Na ₂ CO ₃ ;K ₂ CO ₃ ;BaCO ₃
sulphates	Na ₂ SO ₄ ;(NH ₄) ₂ SO ₄ ;MgSO ₄ ;K ₂ SO ₄ ;Ca ₂ SO ₄
formates	potassium formate
HULIS	HULIS
sugar	glucose
sulfuric acid	sulfuric acid

Table S2. Stretch and bend vibrations of functional groups, assignment to classes of organic and inorganic compounds.

Functional group	Class	Stretch	Bend
O-H	organic acids	4324-3256	894-947,2857-2523
O-H	carbohydrates	3600-3000	
O-H	alcohols	3248-3631	
O-H	HULIS	3300-3700	
O-H	sugars	3432-3534	
C=O	carboxylic acids	1690-1738	1658-1726
C=O	aldehydes	1658-1726	

C=O	amino acids	1653-1668	
C=O	ketones	1708-1728	
C=O	esters	1738-1756	
C=O	lactones	1760-1764	
C=O	quinone	1674	
C=O	HULIS	1734	
C-O	alcohols	1046-1088	
C-O	esters	1016-1290/1374	
H-C=O	aldehydes	2714-2754	
N-H	amino acids	3302-3468	1574-1622
N-H	amines	3382-3402	1582
C-N	amines	1204- 1306	
C-C-H	alkanes	2848-2860/2916-2924;2956-2958	719-729;1371-1378;1456-1466
C=C-H	alkens	3086, 2967;2935-2877	1643
C-C-H	carbohydrates	2888-2895	1371-1454
C-C-H	HULIS	2852-2920	1398-1435
C=C-H	polyaromatics	3028-3090	707-883;1448-1478
C=C	polyaromatics	1584 -1620	
C=C	HULIS	1614	
-NO ₂	organic nitrocompounds	1532-1586/1480-1490	
C-O-C	HULIS	1039;1184;1267	
C-O-C	sugars	1067	
RCOO ⁻	carboxylates	1340-1364/1560	
NO ₃ ⁻	nitrates	1318- 1368	
CO ₃ ²⁻	carbonates	1352-1467	712-713;858-880
NH ₄ ⁺	ammonium	3030-3234	1412
SO ₄ ²⁻	sulphates	597;612;634-638;651-671;706;1008-1032;1056-1085;1100-1103;1182-1188	
SO ₄ ²⁻	sulfuric acids	576-600;629-671;1029-1051;1160-1197	

Symbol slash "/" means symmetric and asymmetric vibrations.

References.

1. Maria, S.F.; Russell, L.M.; Turpin, B.J.; Porcja, R.J. FTIR measurements of functional groups and organic mass in aerosol samples over the Caribbean. *Atmospheric Environment* **2002**, *36*, 5185-5196.
2. Reff, A.; Turpin, B.J.; Offenberg, J.H.; Weisel, C.P.; Zhang, J.; Morandi, M.; Stock, T.; Colome, S.; Winer, A. A functional group characterization of organic PM_{2.5} exposure: Results from the RIOPA study. *Atmospheric Environment* **2007**, *41*, 4585-4598.
3. Coury, C.; Dillner, A.M. A method to quantify organic functional groups and inorganic compounds in ambient aerosols using attenuated total reflectance FTIR spectroscopy and multivariate chemometric techniques. *Atmospheric Environment* **2008**, *42*, 5923-5932.
4. Coates, J. Interpretation of infrared spectra, a practical approach. *Encyclopedia of analytical chemistry: applications, theory and instrumentation* **2006**.