Supplementary material: Coordinates in PCA space for the classical organic solvents.

NAME	CAS	F1	F2	F3	F4
Cluster I: Strong electron pair donor bases					
n-butylamine	109-73-9	-6.0	-8.4	3.0	1.2
diethylamine	109-89-7	-4.2	-8.7	3.9	1.3
n-propylamine	107-10-8	-6.6	-8.3	2.3	0.8
piperidine	110-89-4	-4.5	-8.4	3.8	1.5
pyrrolidine	123-75-1	-5.6	-8.9	3.1	0.6
tributylamine	102-82-9	-5.3	-11.9	5.9	4.5
triethylamine	121-44-8	-5.9	-12.5	5.5	2.9
Cluster II: Weak electron pair donor bases					
acetone	67-64-1	-1.7	-3.2	-3.4	-2.4
DMEU	80-73-9	-2.4	-4.7	-2.1	-2.2
DPMU	7226-23-5	-2.4	-5.9	-0.5	-1.9
N,N-dimethylacetamide	127-19-5	-3.3	-5.5	-2.3	-2.7
N,N-dimethylformamide	68-12-2	-3.8	-4.5	-4.2	-3.1
2,4-dimethylpyridine	108-47-4	-2.4	-6.3	1.3	-0.2
2,6-dimethylpyridine	108-48-5	-2.1	-6.1	1.5	0.1
ethylenediamine	107-15-3	-9.4	-6.1	-2.3	0.3
HMPTA	680-31-9	-2.5	-7.6	1.3	-1.5
N-methyl-pyrrolidin-2-one	872-50-4	-3.1	-5.6	-2.1	-2.7
morpholine	110-91-8	-5.6	-6.0	0.0	-0.3
3-picoline	108-99-6	-2.7	-5.6	0.2	-0.7
4-picoline	108-89-4	-3.0	-5.8	0.2	-0.8
pyridine	110-86-1	-3.5	-4.6	-0.8	-0.6
quinoline	91-22-5	-1.9	-4.0	0.2	-0.2
tetrahydrofuran	109-99-9	-0.5	-5.3	0.8	-0.8
1,1,3,3-tetramethyl urea	632-22-4	-2.4	-6.4	-0.1	-1.9
2,4,6-trimethylpyridine	108-75-8	-2.1	-6.8	2.1	0.3
triethylene glycol	112-27-6	-3.2	-3.2	-2.2	-1.9
Cluster III: Aprotic dipolar					
acetophenone	98-86-2	0.3	-1.6	-1.2	-0.9
benzaldehyde	100-52-7	0.6	-0.8	-1.6	-0.9
2-butanone	78-93-3	-0.5	-3.2	-1.6	-1.5
n-butyl acetate	123-86-4	1.7	-2.4	0.0	-0.3
di-n-butyl ether	142-96-1	1.8	-4.2	2.2	1.5
butyronitrile	109-74-0	-0.2	-0.6	-3.2	-1.4
cyclohexanone	108-94-1	0.2	-3.6	-0.6	-1.2
cyclopentanone	120-92-3	-0.2	-3.0	-1.6	-1.5
DEGDEE	112-36-7	0.6	-3.7	0.6	-0.1
DEGDME	111-96-6	0.8	-2.9	-0.3	-0.5
dibenzyl ether	103-50-4	1.5	-2.1	0.2	-0.4
diethyl carbonate	105-58-8	1.6	-1.5	-1.3	-1.0
diethyl ether	60-29-7	1.3	-4.1	1.4	0.6
di-isopropyl ether	108-20-3	0.6	-5.3	2.5	1.3
1,2-dimethoxyethane	110-71-4	-0.4	-3.5	-1.1	-1.4
3,3-dimethyl-2-butanone	75-97-8	1.1	-3.1	0.0	-0.5
2,6-dimethyl-4-heptanone	108-83-8	2.7	-2.4	1.0	0.8
2,4-dimethyl-3-pentanone	565-80-0	2.3	-2.8	0.6	0.0
1,4-dioxane	123-91-1	-1.4	-3.0	-2.5	-1.7
ethyl acetate	141-78-6	0.8	-2.1	-1.4	-1.0
ethyl benzoate	93-89-0	2.4	-1.1	-0.3	-0.4
ethyl formate	109-94-4	0.0	-0.5	-2.3	-1.1
ethyl propionate	105-37-3	1.7	-2.1	-0.4	-0.5
methyl acetate	79-20-9	-0.3	-1.7	-2.9	-1.5
methyl benzoate	93-58-3	2.1	-0.7	-0.8	-0.6
3-methyl-2-butanone	563-80-4	0.6	-3.0	-0.6	-0.9
Cluster III: Aprotic dipolar continued					
4-methyl-2-pentanone	108-10-1	1.1	-2.9	0.1	-0.3
2-pentanone	107-87-9	0.3	-3.1	-0.5	-0.8
3-pentanone	96-22-0	0.8	-3.0	-0.2	-0.8
pentyl acetate	628-63-7	2.2	-2.2	0.3	0.1
di-n-propyl ether	111-43-3	2.0	-4.1	2.0	1.3
propyl formate	110-74-7	1.2	-0.8	-0.8	-0.6
TEGDME	143-24-8	-0.1	-3.3	-0.4	-0.7
tert-butyl methyl ether	1634-04-4	0.9	-4.7	1.7	0.6
Cluster IV: Aprotic highly dipolar					
acetic anhydride	108-24-7	-0.5	0.5	-4.7	-1.5
acetonitrile	75-05-8	-5.1	2.3	-9.9	-1.2
acetylacetone	123-54-6	-1.7	-0.6	-4.9	-1.8
dimethylsulfoxide	67-68-5	-7.9	-4.3	-8.3	-3.3
N-methylacetamide	79-16-3	-5.6	-1.4	-2.4	0.0
N-methylformamide	123-39-7	-6.9	0.9	-4.4	0.8
methyl formate	107-31-3	-1.4	0.4	-4.1	-1.1
propionitrile	107-12-0	-1.8	0.1	-5.3	-1.6
propylene carbonate	108-32-7	-2.5	1.2	-5.9	-1.1
sulfolane	126-33-0	-3.9	-0.1	-9.0	-3.0
Cluster V: Apolar					
benzene	71-43-2	5.6	1.6	-0.8	-0.7
bromobenzene	108-86-1	5.2	2.5	-1.2	0.0
1-bromobutane	109-65-9	6.1	1.4	-0.5	-0.2
bromoethane	74-96-4	4.8	1.9	-1.7	-0.9
carbon disulfide	75-15-0	7.4	3.2	0.2	6.6
carbon tetrachloride	56-23-5	7.9	1.6	0.3	1.8
chlorobenzene	108-90-7	5.8	2.0	-0.4	-0.9
1-chlorobutane	109-69-3	6.2	1.3	-0.2	-0.1
1-chloropropane	540-54-5	5.9	1.3	-0.4	-0.5
2-chloropropane	75-29-6	5.6	1.3	-0.7	-0.8
cis-decaline	91-17-8	8.4	1.8	0.6	3.7
cyclohexane	110-82-7	8.4	1.8	0.6	3.5
cyclohexene	110-83-8	7.1	0.9	0.6	1.8
cyclopentane	287-92-3	8.4	1.7	0.7	3.3
n-decane	124-18-5	8.3	1.8	0.6	3.5
o-dichlorobenzene	95-50-1	6.0	2.2	-0.3	-0.8
1,1-dichloroethylene	75-35-4	6.1	2.5	0.0	-0.7
m-dichlorobenzene	541-73-1	5.8	2.4	-0.2	-1.0
N,N-dimethylaniline	121-69-7	5.3	1.3	-1.0	-0.8
diphenyl ether	101-84-8	5.3	1.5	-0.6	-0.5
fluorobenzene	462-06-6	5.7	1.7	-0.3	-1.4
n-heptane	142-82-5	8.3	1.8	0.6	3.4
n-hexane	110-54-3	8.3	1.7	0.5	3.3
iodobenzene	591-50-4	5.4	2.6	-0.8	0.6
iodoethane	75-03-6	4.8	2.3	-1.5	0.4
mesitylene	108-67-8	6.7	1.2	0.0	0.4
iso-octane	540-84-1	8.3	1.7	0.5	3.2
n-octane	111-65-9	8.3	1.8	0.6	3.4
n-pentane	109-66-0	8.3	1.7	0.5	3.3
phenetole	103-73-1	4.2	0.3	-0.4	-0.4
styrene	100-42-5	5.6	1.7	-0.8	-0.8
tetrachloroethylene	127-18-4	8.0	1.6	0.2	1.8
toluene	108-88-3	6.1	1.4	-0.5	-0.3
1,1,1-trichloroethane	71-55-6	**6.3**	**1.9**	**-0.1**	**-0.6**
Cluster V: Apolar continued					
trichloroethylene	79-01-6	5.1	3.8	0.6	-1.3
m-xylene	108-38-3	6.5	1.2	-0.2	0.0
o-xylene	95-47-6	6.3	1.2	-0.3	-0.1
p-xylene	106-42-3	6.5	1.2	-0.2	0.0
Cluster VI: Asymetric halogenated hydrocarbons					
aniline	62-53-3	-2.0	3.3	0.5	-1.4
anisole	100-66-3	3.7	0.6	-0.9	-0.8
benzonitrile	100-47-0	0.5	0.8	-2.8	-0.6
chloroform	67-66-3	2.2	6.0	0.9	-4.2
1,1-dichloroethane	75-34-3	4.2	3.1	0.0	-2.1
1,2-dichloroethane	107-06-2	3.5	3.1	-0.2	-2.0
Z-1,2-dichloroethylene	156-59-2	4.0	3.8	0.3	-2.7
dichloromethane	75-09-2	2.9	4.4	0.6	-3.3
nitrobenzene	98-95-3	2.5	1.7	-1.7	-0.1
nitroethane	79-24-3	0.1	3.1	-3.5	0.3
nitromethane	75-52-5	-2.0	5.1	-3.5	2.2
1,1,2,2-tetrachloroethane	79-34-5	2.7	5.4	0.7	-3.7
Cluster VII: Amphiprotic					
1-butanol	71-36-3	-2.8	1.9	3.6	1.1
2-butanol	78-92-2	-2.8	1.0	3.1	1.1
benzyl alcohol	100-51-6	-3.4	4.2	2.7	-1.3
tert-butyl alcohol	75-65-0	-2.7	0.9	3.2	1.1
cyclohexanol	108-93-0	-2.2	0.8	3.6	1.2
ethanol	64-17-5	-4.6	2.2	1.9	1.3
1-hexanol	111-27-3	-2.1	1.8	4.1	1.2
isobutyl alcohol	78-83-1	-2.7	2.0	3.5	1.0
2-methyl-2-butanol	75-85-4	-2.3	0.6	3.5	1.2
3-methyl-1-butanol	123-51-3	-2.5	1.8	3.8	1.0
tetraethylene glycol	112-60-7	-4.2	3.8	2.9	0.2
1-pentanol	71-41-0	-2.4	1.8	3.9	1.1
2-pentanol	6032-29-7	-2.4	1.3	3.8	1.2
3-pentanol	584-02-1	-1.9	1.5	3.9	1.0
1-propanol	71-23-8	-3.5	2.1	3.0	1.2
2-propanol	67-63-0	-3.5	1.7	2.9	1.2
1-octanol	111-87-5	-1.2	0.8	4.0	1.2
Cluster VIII: Polar protic					
2-aminoethanol	141-43-5	-8.4	-0.1	-2.4	1.6
ethylene glycol	107-21-1	-7.6	5.2	-0.9	2.6
diethylene glycol	111-46-6	-5.8	1.6	-0.6	-0.1
trimethylene glycol	504-63-2	-5.9	2.5	1.1	1.4
glycerol	56-81-5	-7.4	5.7	-0.4	2.0
propylene glycol	57-55-6	-5.5	3.9	1.3	1.4
methanol	67-56-1	-6.5	3.7	0.5	2.3
2-methoxyethanol	109-86-4	-4.5	1.1	0.2	-0.6
furfuryl alcohol	98-00-0	-4.5	4.8	1.8	-0.9
Cluster IX: Organic acidic compounds					
acetic acid	64-19-7	-7.2	8.5	2.3	-0.8
m-cresol	108-39-4	-5.2	11.1	5.0	-5.3
phenol	108-95-2	-5.9	11.8	5.1	-5.5
trifluoroacetic acid	76-05-1	-10.8	18.9	7.3	-11.1
2,2,2-trifluoroethanol	75-89-8	-5.5	10.3	4.9	-3.7
Cluster X: Polar structured					
formamide	75-12-7	-11.6	8.1	-7.5	7.9
water	7732-18-5	-16.7	17.2	-5.3	15.8