Supporting Information for *ChemPhysChem* 200400171

Accurate pK_a Determination for a Heterogeneous Group of Organic Molecules

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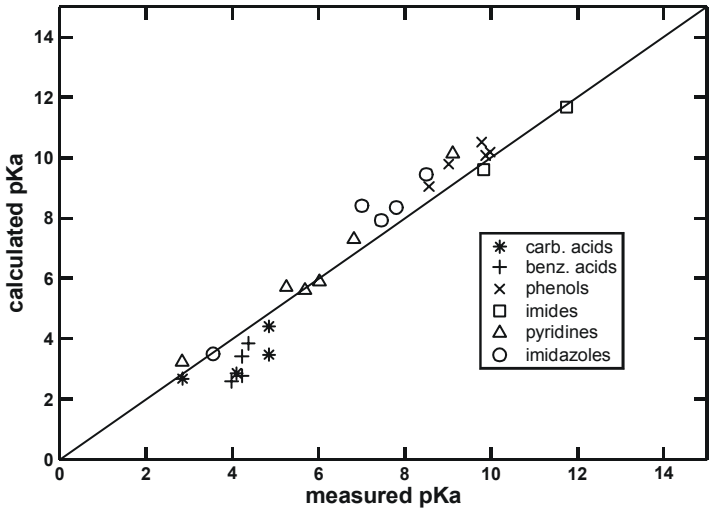
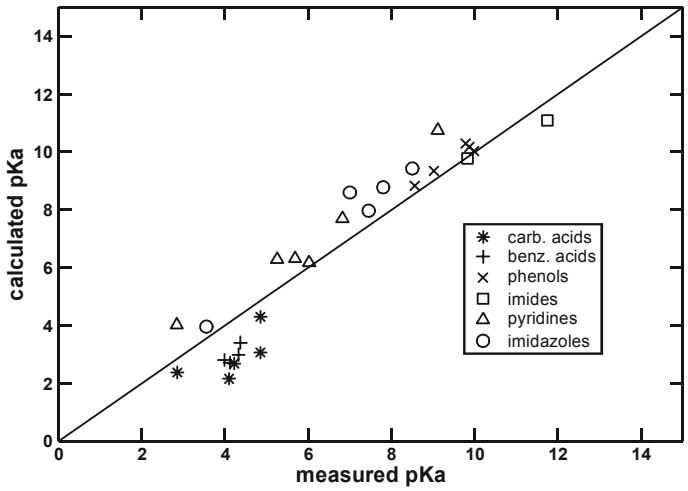
Figure S1: Correlation diagram of experimental and calculated pK_a values of the 26 compounds considered using Becke($^1/_2$).



The computed pK_a values are based on electronic energies E_0 obtained with Becke($^1/_2$)/cc-pvqz. Atomic partial charges used for computation of solvation energies were calculated Becke($^1/_2$)/6-31G++** on optimized geometries with The pK_a values displayed in this Figure were calculated with a $\Delta G_{solv}(H^+)$ value of –260.72 kcal/mol yielding an RMS deviation of 0.76 pK_a units .

Figure S2: Correlation diagram of experimental and calculated pK_a values of the 26 compounds considered using B3lYP.



The computed pK_a values are based on electronic energies E_0 obtained with B3LYP-pvqz. Atomic partial charges used for computation of solvation energies were calculated with B3LYP/6-31G++** on optimized geometries. The pK_a values displayed in this Figure were calculated with a $\Delta G_{solv}(H^+)$ value of –264.01 kcal/mol yielding an RMS deviation of 1.01 pK_a units .

Table S1: Comparison of calculated and experimental pK_a values. The PA values were calculated with Becke($^1/_2$)/cc-pvqz. For the calculation of $\Delta\Delta G_{solv}$ atomic partial charges generated with Becke($^1/_2$)/6-31++G** were applied. The pK_a values listed in this Table were used for the correlation diagram in Figure S1.

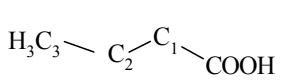
compound	PA	$\Delta\Delta G_{solv}$	calc. pK_a	expl. pK_a	ΔpK_a
propionic acid	344.84	-71.89	3.50	4.85	-1.35
butyric acid	345.02	-70.79	4.44	4.85	-0.41
2-chloropropionic acid	337.10	-65.22	2.71	2.85	-0.14
3-chloropropionic acid	335.31	-63.20	2.88	4.10	-1.22
benzoic acid	338.95	-67.09	2.70	4.22	-1.52
p-methylbenzoic acid	340.27	-66.82	3.88	4.37	-0.49
m-methylbenzoic acid	339.70	-66.93	3.45	4.22	-0.77
p-chlorobenzoic acid	334.65	-62.78	2.71	3.98	-1.27
phenol	347.71	-65.63	10.21	9.98	0.23
m-aminophenol	349.65	-67.73	10.10	9.87	0.23
o-aminophenol	348.57	-66.04	10.55	9.78	0.77
m-chlorophenol	340.19	-58.67	9.81	9.02	0.79
o-chlorophenol	343.24	-62.71	9.08	8.56	0.52
glutarimide	349.48	-65.38	11.71	11.75	-0.04
glutaconimide	346.81	-65.52	9.63	9.83	-0.20
pyridine	220.89	-55.10	5.73	5.25	0.48
2-methyl-pyridine	225.21	-50.63	5.63	5.68	-0.05
4-methyl-pyridine	225.55	-50.68	5.92	6.02	-0.10
2-amino-pyridine	226.20	-51.95	7.32	6.82	0.50
4-amino-pyridine	234.19	-47.80	10.15	9.11	1.04
3-chlor-pyridine	215.13	-57.49	3.26	2.84	0.42
imidazole	224.33	-55.32	8.43	7.00	1.43
2-methylimidazole	229.75	-49.84	8.39	7.80	0.59
4-methylimidazole	228.04	-50.96	7.95	7.45	0.50
2-aminoimidazole	233.05	-48.01	9.47	8.50	0.97
2-chloroimidazole	218.42	-54.57	3.53	3.55	-0.02

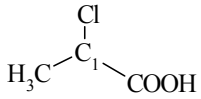
Table S2: Comparison of calculated and experimental pK_a values. The PA values were calculated with B3LYP/cc-pvqz. For the calculation of $\Delta\Delta G_{solv}$ atomic partial charges generated with B3LYP/6-31++G** were applied. The pK_a values listed in this Table were used for the correlation diagram in Figure S2.

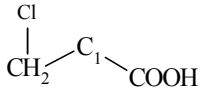
compound	PA	$\Delta\Delta G_{solv}$	calc. pK_a	expl. pK_a	ΔpK_a
propionic aicd	347.36	-71.44	3.09	4.85	-1.76
butyric acid	347.97	-70.35	4.34	4.85	-0.51
2-chloropropionic acid	339.71	-64.71	2.41	2.85	-0.44
3-chloropropionic acid	337.36	-62.66	2.19	4.10	-1.91
benzoic acid	341.81	-66.37	2.73	4.22	-1.49
p-methylbenzoic acid	342.36	-65.96	3.45	4.37	-0.92
m-methylbenzoic acid	341.71	-66.12	2.85	4.22	-1.37
p-chlorobenzoic acid	337.69	-62.11	2.84	3.98	-1.14
phenol	350.43	-65.01	10.07	9.98	0.09
m-aminophenol	352.61	-67.00	10.22	9.87	0.35
o-aminophenol	351.11	-65.35	10.33	9.78	0.55
m-chlorophenol	342.76	-58.28	9.39	9.02	-0.37
o-chlorophenol	345.89	-62.11	8.86	8.56	0.30
glutarimide	351.30	-64.45	11.13	11.75	-0.62
glutaconimide	349.60	-64.53	9.82	9.83	-0.01
pyridine	224.78	-55.54	6.32	5.25	1.07
2-methylpyridine	229.23	-51.13	6.36	5.68	0.68
4-methylpyridine	229.00	-51.16	6.21	6.02	0.19
2-aminopyridine	230.01	-52.22	7.74	6.82	0.92
4-aminopyridine	238.17	-48.21	10.78	9.11	1.67
3-chloropyridine	219.88	-57.36	4.06	2.84	1.22
imidazole	227.57	-55.90	8.64	7.00	1.64
2-methylimidazole	233.24	-50.46	8.81	7.80	1.01
4-methylimidazole	231.09	-51.51	8.00	7.45	0.56
2-aminoimidazole	235.87	-48.72	9.47	8.50	0.97
2-chloroimidazole	222.27	-54.88	3.99	3.55	0.45

Tables S3(a-e): Influence of basis set and DFT functional on solvation energies. All energies are given in kcal/mol.
Table S3a: Dependence of basis set and DFT functional on $\Delta G_{solv}(AH)$, $\Delta G_{solv}(A^-)$ and $\Delta\Delta G_{solv}$ for carboxylic acids and benzoic acids.

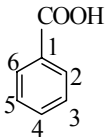
Basis set	butyric acid			2-chloropropionic acid			3-chloropropionic acid		
	anion	neutral	$\Delta\Delta G_{solv}$	anion	neutral	$\Delta\Delta G_{solv}$	anion	neutral	$\Delta\Delta G_{solv}$
Becke($^1/_2$)6-31G**	-79.95	-11.45	-68.50	-75.17	-11.94	-63.23	-74.54	-13.61	-60.93
Becke($^1/_2$)6-31++G**	-83.36	-12.56	-70.79	-77.91	-12.69	-65.22	-77.87	-14.67	-63.20
Becke($^1/_2$)6-311++G**	-83.26	-12.50	-70.76	-77.84	-12.65	-65.19	-77.83	-14.53	-63.30
Becke($^1/_2$)6-311+G*	-83.51	-13.03	-70.48	-77.91	-13.17	-64.73	-77.94	-15.16	-62.77
Becke($^1/_2$)6-311G	-83.12	-15.01	-68.11	-78.47	-15.77	-62.70	-77.65	-17.49	-60.16
B3LYP/6-31G**	-78.20	-10.44	-67.76	-73.51	-10.97	-62.54	-72.36	-12.41	-59.95
B3LYP/6-31++G**	-82.01	-11.66	-70.35	-76.49	-11.78	-64.71	-76.22	-13.56	-62.66

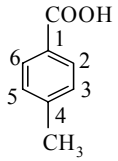


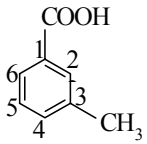




basis set	benzoic acid			p-methylbenzoic acid			m-methylbenzoic acid			p-chlorobenzoic acid		
	anion	neutral	$\Delta\Delta G_{solv}$	anion	neutral	$\Delta\Delta G_{solv}$	anion	neutral	$\Delta\Delta G_{solv}$	anion	neutral	$\Delta\Delta G_{solv}$
Becke($^1/_2$)6-31G**	-78.13	-13.30	-64.83	-77.58	-13.67	-63.91	-77.52	-13.09	-64.43	-73.76	-13.04	-60.72
Becke($^1/_2$)6-31++G**	-81.32	-14.23	-67.09	-81.42	-14.61	-66.81	-80.96	-14.03	-66.93	-76.53	-13.76	-62.77
Becke($^1/_2$)6-311++G**	-81.46	-14.32	-67.14	-81.62	-14.77	-66.85	-81.14	-14.16	-66.98	-76.63	-13.54	-63.09
Becke($^1/_2$)6-311+G**	-81.52	-14.32	-67.19	-81.51	-14.75	-66.75	-81.19	-14.17	-67.02	-76.75	-13.79	-62.95
Becke($^1/_2$)6-311+G*	-81.92	-15.12	-66.79	-81.82	-15.51	-66.30	-81.50	-14.89	-66.60	-77.04	-14.48	-62.56
Becke($^1/_2$)6-311G	-81.16	-16.40	-64.75	-81.43	-16.77	-64.65	-81.36	-16.58	-64.77	-76.04	-16.25	-59.78
B3LYP/6-31G**	-75.42	-11.87	-63.55	-75.35	-12.27	-63.08	-75.11	-11.67	-63.44	-70.79	-11.61	-59.17
B3LYP/6-31++G**	-79.25	-12.88	-66.37	-79.21	-13.25	-65.96	-78.82	-12.70	-66.11	-74.69	-12.58	-62.11







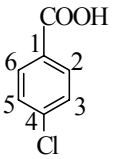


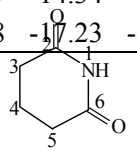
Table S3b: Dependence of basis set and DFT functional on $\Delta G_{solv}(AH)$, $\Delta G_{solv}(A^-)$ and $\Delta\Delta G_{solv}$ for substituted phenols.

basis set	phenol			m-aminophenol			o-aminophenol		
	anion	neutral	$\Delta\Delta G_{solv}$	anion	neutral	$\Delta\Delta G_{solv}$	anion	neutral	$\Delta\Delta G_{solv}$
Becke($^1/_2$)6-31G**	-75.15	-10.71	-64.44	-83.04	-16.92	-66.12	-79.94	-15.53	-64.41
Becke($^1/_2$)6-31++G**	-77.44	-11.81	-65.63	-86.31	-18.58	-67.73	-83.15	-17.11	-66.03
Becke($^1/_2$)6-311++G**	-78.02	-11.93	-66.08	-86.42	-18.50	-67.91	-83.28	-16.86	-66.42
Becke($^1/_2$)6-311+G**	-77.99	-11.92	-66.06	-86.53	-18.53	-67.99	-83.23	-16.93	-66.29
Becke($^1/_2$)6-311+G*	-78.69	-13.09	-65.60	-87.92	-20.25	-67.67	-84.69	-18.55	-66.14
Becke($^1/_2$)6-311G	-77.93	-13.91	-64.02	-86.84	-20.70	-66.13	-83.75	-18.49	-65.25
B3LYP/6-31G**	-73.20	-9.80	-63.40	-80.50	-15.32	-65.17	-77.55	-14.06	-63.49
B3LYP/6-31++G**	-75.54	-10.53	-65.01	-83.75	-16.74	-67.00	-80.68	-15.33	-65.35

basis set	m-chlorophenol			o-chlorophenol		
	anion	neutral	$\Delta\Delta G_{solv}$	anion	neutral	$\Delta\Delta G_{solv}$
Becke($^1/_2$)6-31G**	-67.30	-10.01	-57.29	-68.97	-7.50	-61.47
Becke($^1/_2$)6-31++G**	-69.49	-10.82	-58.66	-70.91	-8.20	-62.71
Becke($^1/_2$)6-311++G**	-70.18	-10.85	-59.33	-71.45	-8.24	-63.21
Becke($^1/_2$)6-311+G**	-69.93	-10.84	-59.09	-71.40	-8.23	-63.16
Becke($^1/_2$)6-311+G*	-70.37	-11.84	-58.52	-71.83	-9.10	-62.72
Becke($^1/_2$)6-311G	-69.61	-13.13	-56.47	-71.62	-10.63	-60.99
B3LYP/6-31G**	-65.68	-8.98	-56.69	-67.25	-6.72	-60.52
B3LYP/6-31++G**	-68.07	-9.79	-58.28	-69.41	-7.29	-62.11

Table S3c: Dependence of basis set and DFT functional on $\Delta G_{solv}(AH)$, $\Delta G_{solv}(A^-)$ and $\Delta\Delta G_{solv}$ for imides.

basis set	glutarimide			glutaconimide		
	anion	neutral	$\Delta\Delta G_{solv}$	anion	neutral	$\Delta\Delta G_{solv}$
Becke($^1/_2$)6-31G**	-79.01	-15.93	-63.08	-80.45	-17.10	-63.35
Becke($^1/_2$)6-31++G**	-83.88	-18.51	-65.37	-85.47	-19.94	-65.52
Becke($^1/_2$)6-311++G**	-83.49	-18.35	-65.13	-85.50	-19.75	-65.74
Becke($^1/_2$)6-311+G**	-83.74	-18.49	-65.25	-85.60	-19.95	-65.65
Becke($^1/_2$)6-311+G*	-83.82	-18.56	-65.26	-85.64	-20.09	-65.55
Becke($^1/_2$)6-311G	-84.68	-19.89	-64.79	-86.80	-21.52	-65.28
B3LYP/6-31G**	-76.39	-14.34	-62.05	-77.67	-15.47	-62.20
B3LYP/6-31++G**	-81.68	-17.23	-64.45	-82.89	-18.36	-64.53



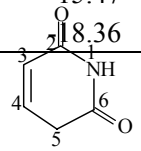
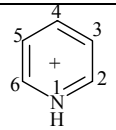
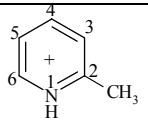
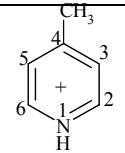
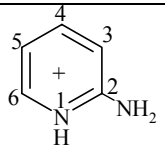
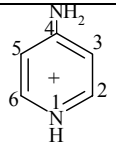
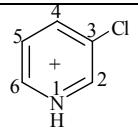


Table S3d: Dependence of basis set and DFT functional on $\Delta G_{solv}(AH^+)$, $\Delta G_{solv}(A)$ and $\Delta\Delta G_{solv}$ for substituted pyridines

basis set	pyridine			2-methylpyridine			4-methylpyridine		
	neutral	cation	$\Delta\Delta G_{solv}$	neutral	cation	$\Delta\Delta G_{solv}$	neutral	cation	$\Delta\Delta G_{solv}$
Becke($^1/_2$)6-31G**	-7.92	-63.87	55.95	-7.38	-59.08	51.72	-8.27	-60.01	51.74
Becke($^1/_2$)6-31++G**	-8.86	-63.96	55.09	-8.32	-58.95	50.63	-9.28	-59.96	50.68
Becke($^1/_2$)6-311++G**	-9.00	-63.84	54.84	-8.48	-58.86	50.38	-9.46	-62.89	53.43
Becke($^1/_2$)6-311+G**	-9.00	-63.91	54.91	-8.50	-58.88	50.37	-9.45	-62.93	53.47
Becke($^1/_2$)6-311+G*	-9.20	-64.16	54.95	-8.76	-59.18	50.42	-9.61	-60.21	50.59
Becke($^1/_2$)6-311G	-10.06	-64.12	54.05	-9.37	-59.16	49.79	-10.45	-60.25	49.80
B3LYP/6-31G**	-6.92	-63.56	56.63	-6.59	-58.56	51.97	-7.31	-59.75	52.43
B3LYP/6-31++G**	-7.99	-63.53	55.53	-7.43	-58.56	51.13	-8.36	-59.53	51.16

basis set	2-aminopyridine			4-aminopyridine			3-chloropyridine		
	neutral	cation	$\Delta\Delta G_{solv}$	neutral	cation	$\Delta\Delta G_{solv}$	neutral	cation	$\Delta\Delta G_{solv}$
Becke($^1/_2$)6-31G**	-12.02	-64.03	52.01	-14.38	-62.76	48.38	-5.86	-64.39	58.53
Becke($^1/_2$)6-31++G**	-12.50	-64.45	51.94	-15.37	-63.17	47.79	-6.57	-64.06	57.49
Becke($^1/_2$)6-311++G**	-12.49	-64.25	51.75	-15.34	-62.89	47.55	-6.50	-63.79	57.29
Becke($^1/_2$)6-311+G**	-12.47	-64.27	51.79	-15.32	-62.93	47.60	-6.52	-63.80	57.27
Becke($^1/_2$)6-311+G*	-13.08	-64.93	51.85	-15.95	-63.60	47.64	-6.61	-64.00	57.39
Becke($^1/_2$)6-311G	-15.02	-64.85	49.82	-17.99	-63.45	45.46	-7.83	-65.01	57.18
B3LYP/6-31G**	-10.67	-63.09	52.42	-12.87	-61.81	48.93	-5.22	-63.82	58.60
B3LYP/6-31++G**	-11.25	-63.47	52.22	-13.96	-62.17	48.20	-5.96	-63.32	57.35

basis set	imidazole			2-methylimidazole			4-methylimidazole			2-aminoimidazole			2-chloroimidazole		
	neutral	cation	$\Delta\Delta G_{solv}$	neutral	cation	$\Delta\Delta G_{solv}$	neutral	cation	$\Delta\Delta G_{solv}$	neutral	cation	$\Delta\Delta G_{solv}$	neutral	cation	$\Delta\Delta G_{solv}$
Becke($^1/_2$)6-31G**	-13.22	-69.21	55.99	-13.22	-63.61	50.39	-12.66	-64.42	51.76	-19.70	-68.54	48.84	-10.17	-65.15	54.98
Becke($^1/_2$)6-31++G**	-13.86	-69.18	55.32	-13.76	-63.60	49.83	-13.35	-64.31	50.95	-20.98	-68.99	48.01	-10.58	-65.15	54.57
Becke($^1/_2$)6-311++G**	-13.73	-69.13	55.39	-13.74	-63.57	49.83	-13.20	-64.24	51.04	-20.79	-68.85	48.06	-10.28	-65.07	54.79
Becke($^1/_2$)6-311+G**	-13.73	-69.13	55.39	-13.75	-63.56	49.81	-13.19	-64.23	51.04	-20.76	-68.80	48.04	-10.53	-65.03	54.49
Becke($^1/_2$)6-311+G*	-14.21	-69.52	55.31	-14.22	-64.08	49.86	-13.63	-64.67	51.04	-21.88	-69.71	47.82	-10.61	-65.36	54.75
Becke($^1/_2$)6-311G	-15.21	-69.32	54.11	-15.15	-63.78	48.63	-14.64	-64.61	49.96	-22.79	-69.56	46.76	-12.41	-66.01	53.59
B3LYP/6-31G**	-11.88	-68.66	56.77	-11.70	-63.08	51.38	-11.40	-63.80	52.39	-17.98	-67.57	49.58	-9.32	-64.67	55.35
B3LYP/6-31++G**	-12.68	-68.58	55.89	-12.62	-63.08	50.46	-12.19	-63.70	51.51	-19.26	-67.98	48.72	-9.73	-64.61	54.88

Table S3e: Dependence of basis set and DFT functional on $\Delta G_{solv}(AH^+)$, $\Delta G_{solv}(A^-)$ and $\Delta\Delta G_{solv}$ for substituted imidazoles

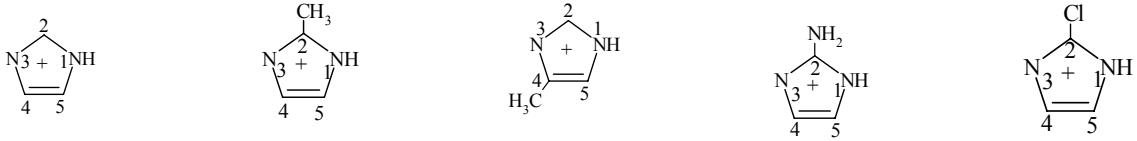
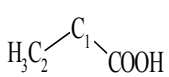
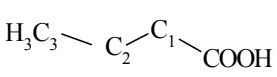


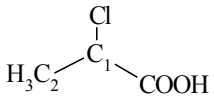
Table S4 (a-f): Atomic partial charges for all 32 compounds listed in Figure 1. The charges were generated with Becke($^1/_2$)/6-31G** and RESP on optimized geometries. The $\Delta\Delta G_{solv}$ values depicted in the **Table S4** were employed for pK_a calculations (see **Table 2**), with the exception from the data of **Table S4e** (unmodified point charges and solvation energies for methylated phenols).

Table S4a: Atomic partial charges, ΔG_{solv} (AH), ΔG_{solv} (A^-) and $\Delta\Delta G_{solv}$ for substituted carboxylic acids.

propionic acid			butyric acid			2-chloropropionic acid			3-chloropropionic acid		
	neutral	anion		neutral	anion		neutral	anion		neutral	anion
C	0.6474	0.6948	C	0.6158	0.6931	C	0.6351	0.7025	C	0.6804	0.7120
O	-0.5608	-0.7449	O	-0.5247	-0.7465	O	-0.5095	-0.7235	O	-0.5486	-0.7443
O_H	-0.5832	-0.7775	O_H	-0.5835	-0.7554	O_H	-0.5540	-0.7270	O_H	-0.6059	-0.7463
H	0.4294		H	0.4256		H	0.4321		H	0.4407	
C_1	-0.0131	0.0247	C_1	-0.1687	-0.1490	C_1	-0.0169	0.1391	C_1	-0.0536	-0.0719
H_{11}	0.0426	-0.0375	H_{11}	0.0550	-0.0159	H_{11}	0.1148	0.0359	H_{11}	0.0696	0.0086
H_{12}	0.0479	-0.0319	H_{12}	0.0817	0.0095	Cl_1	-0.1635	-0.3450	H_{12}	0.0767	0.0165
C_2	-0.2072	-0.1748	C_2	0.1869	0.2116	C_2	-0.2389	-0.2619	C_2	-0.1621	0.0164
H_{21}	0.0672	0.0304	H_{21}	-0.0050	-0.0483	H_{21}	0.1006	0.0780	H_{21}	0.1388	0.0790
H_{22}	0.0684	0.0351	H_{22}	-0.0037	-0.0287	H_{22}	0.0971	0.0259	H_{22}	0.1424	0.0860
H_{23}	0.0612	-0.0182	C_3	-0.3340	-0.2957	H_{23}	0.1029	0.0759	Cl_2	-0.1785	-0.3561
			H_{31}	0.0838	0.0322						
			H_{32}	0.0832	0.0498						
			H_{33}	0.0872	0.0435						







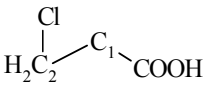


Table S4b: Atomic partial charges, $\Delta G_{solv}(AH)$, $\Delta G_{solv}(A^-)$ and $\Delta\Delta G_{solv}$ for substituted benzoic acids.

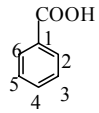
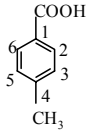
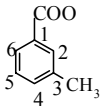
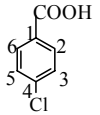
benzoic acid			p-methylbenzoic acid			m-methylbenzoic acid			p-chlorobenzoic acid		
	neutral	anion		neutral	anion		neutral	anion		neutral	anion
C	0.6086	0.6503	C	0.6370	0.6752	C	0.6377	0.6714	C	0.6218	0.6694
O	-0.5252	-0.7133	O	-0.5408	-0.7186	O	-0.5314	-0.7174	O	-0.5292	-0.7178
O_H	-0.5748	-0.7136	O_H	-0.5833	-0.7195	O_H	-0.5813	-0.7190	O_H	-0.5770	-0.7182
H	0.4290		H	0.4270		H	0.4275		H	0.4297	
C_1	0.0175	0.0171	C_1	-0.0370	-0.0229	C_1	0.0207	0.0419	C_1	0.0129	0.0025
C_2	-0.1392	-0.1318	C_2	-0.1232	-0.1112	C_2	-0.2724	-0.2846	C_2	-0.1742	-0.1540
C_3	-0.1104	-0.1444	C_3	-0.2366	-0.2830	C_3	0.2787	0.2584	C_3	-0.0466	-0.1286
C_4	-0.0983	-0.1528	C_4	0.2949	0.2379	C_4	-0.2316	-0.3067	C_4	0.0335	0.0827
C_5	-0.1194	-0.1444	C_5	-0.2559	-0.2887	C_5	-0.1044	-0.1163	C_5	-0.0565	-0.1284
C_6	-0.1342	-0.1324	C_6	-0.1087	-0.1129	C_6	-0.1742	-0.1810	C_6	-0.1680	-0.1539
H_2	0.1383	0.1022	H_2	0.1458	0.1099	H_2	0.1644	0.1375	H_2	0.1570	0.1247
H_3	0.1224	0.0857	H_3	0.1437	0.1162	C_3	-0.4449	-0.3875	H_3	0.1157	0.0996
						H_{31}	0.1319	0.0975			
						H_{32}	0.1214	0.0816			
						H_{33}	0.1319	0.0975			
H_4	0.1212	0.0895	C_4	-0.4478	-0.3796	H_4	0.1458	0.1218	Cl_4	-0.0955	-0.2023
			H_{41}	0.1276	0.0898						
			H_{42}	0.1326	0.0902						
			H_{43}	0.1326	0.0902						
H_5	0.1229	0.0860	H_5	0.1444	0.1168	H_5	0.1296	0.0911	H_5	0.1160	0.0995
H_6	0.1412	0.1020	H_6	0.1478	0.1104	H_6	0.1504	0.1136	H_6	0.1602	0.1248
											

Table S4c: Atomic partial charges, $\Delta G_{solv}(AH)$, $\Delta G_{solv}(A^-)$ and $\Delta\Delta G_{solv}$ for substituted phenols.

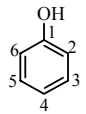
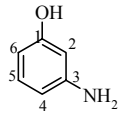
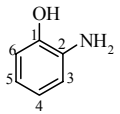
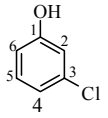
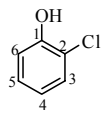
	phenol			m-amino-phenol			o-amino-phenol			m-chloro-phenol			o-chloro-phenol	
	neutr.	anion		neutr.	anion		neutr.	anion		neutr.	anion		neutr.	anion
C_1	0.3999	0.5941	C_1	0.4514	0.6563	C_1	0.2338	0.4607	C_1	0.3838	0.5969	C_1	0.3940	0.5809
C_2	-0.3324	-0.4062	C_2	-0.4816	-0.6602	C_2	0.3913	0.2119	C_2	-0.2985	-0.4287	C_2	-0.0999	-0.0955
C_3	-0.0490	-0.0531	C_3	0.5603	0.6114	C_3	-0.3303	-0.2839	C_3	0.1126	0.2106	C_3	-0.0570	-0.0954
C_4	-0.1869	-0.3503	C_4	-0.4201	-0.5692	C_4	-0.1492	-0.3024	C_4	-0.1395	-0.3595	C_4	-0.2027	-0.3459
C_5	-0.0889	-0.0530	C_5	0.0029	-0.0096	C_5	-0.1495	-0.1319	C_5	-0.1279	-0.0610	C_5	-0.0897	-0.0533
C_6	-0.2479	-0.4067	C_6	-0.4478	-0.4980	C_6	-0.3175	-0.4382	C_6	-0.2554	-0.4322	C_6	-0.2750	-0.4490
O	-0.5717	-0.7458	O	-0.5708	-0.7449	O	-0.5712	-0.7325	O	-0.5654	-0.7185	O	-0.5341	-0.7019
H	0.4086		H	0.4098		H	0.4166		H	0.4210		H	0.3846	
H_2	0.1472	0.0970	H_2	0.1645	0.1400	N_2	-0.9403	-0.9272	H_2	0.1481	0.1324	Cl_2	-0.0990	-0.2525
						H_{21}	0.3985	0.3620						
						H_{22}	0.4208	0.3670						
H_3	0.1169	0.0673	N_3	-0.9949	-1.043	H_3	0.1702	0.1128	Cl_3	-0.1188	-0.2636	H_3	0.1325	0.0957
			H_{31}	0.4194	0.3857									
			H_{32}	0.4127	0.3923									
H_4	0.1211	0.0924	H_4	0.1252	0.0770	H_4	0.1336	0.1002	H_4	0.1449	0.0894	H_4	0.1298	0.0811
H_5	0.1601	0.0673	H_5	0.1639	0.1129	H_5	0.1309	0.0811	H_5	0.1716	0.1163	H_5	0.1754	0.1245
H_6	0.1230	0.0970	H_6	0.2048	0.1485	H_6	0.1623	0.1205	H_6	0.1235	0.1179	H_6	0.1411	0.1113
														

Table S4d: Atomic partial charges for glutarimide and glutacoimide

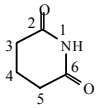
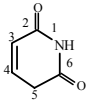
	Glutarimide			Glutaconimide	
	Neutral	Anion		neutral	Anion
N_1	-0.6001	-0.8874	N_1	-0.6393	-0.9206
C_2	0.6397	0.8057	C_2	0.7688	0.9217
C_3	-0.2493	-0.3148	C_3	-0.4414	-0.4996
C_4	0.0909	0.1795	C_4	0.0217	0.0144
C_5	-0.2512	-0.3121	C_5	-0.1965	-0.2850
C_6	0.6411	0.8031	C_6	0.6855	0.8476
H_1	0.3558		H_1	0.3579	
O_2	-0.5204	-0.6890	O_2	-0.5327	-0.7071
H_{3a}	0.0862	0.0550	H_3	0.1895	0.1398
H_{3b}	0.0974	0.0360			
H_{4a}	0.0230	-0.0274	H_4	0.1208	0.0598
H_{4b}	0.0235	-0.0509			
H_{5a}	0.0872	0.0556	H_5	0.1041	0.0625
H_{5b}	0.0978	0.0326	H_5	0.1020	0.0618
O_6	-0.5218	-0.6858	O_6	-0.5405	-0.6951
					

Table S4e: Atomic partial charges, $\Delta G_{solv}(AH)$, $\Delta G_{solv}(A^-)$ and $\Delta\Delta G_{solv}$ for substituted pyridines.

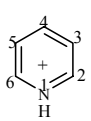
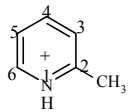
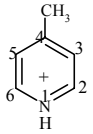
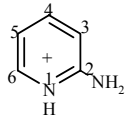
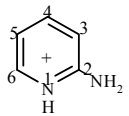
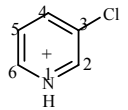
pyridine			2-CH_3-pyridine			4-CH_3-pyridine			2-NH_2-pyridine			4-NH_2-pyridine			3-Cl-pyridine	
	cation	neutral		cation	neutral		cation	neutral		cation	neutral		cation	neutral		cation	neutral
N_1	-0.1275	-0.6461	N_1	-0.2008	-0.6670	N_1	-0.1617	-0.6616	N_1	-0.3246	-0.6678	N_1	-0.2256	-0.6777	N_1	-0.1584	-0.5154
C_2	0.0390	0.4651	C_2	0.3837	0.7603	C_2	0.0456	0.4705	C_2	0.6991	0.8244	C_2	0.0764	0.4695	C_2	0.1510	0.3250
C_3	-0.1194	-0.4670	C_3	-0.2282	-0.5250	C_3	-0.2265	-0.6036	C_3	-0.3695	-0.5562	C_3	-0.3630	-0.6459	C_3	-0.0971	-0.0874
C_4	0.0562	0.2027	C_4	0.0511	0.1732	C_4	0.3951	0.5926	C_4	0.0925	0.1659	C_4	0.6871	0.7113	C_4	0.1478	0.0058
C_5	-0.1197	-0.4672	C_5	-0.1601	-0.4548	C_5	-0.2274	-0.6040	C_5	-0.2101	-0.4696	C_5	-0.3630	-0.6450	C_5	-0.1672	-0.2187
C_6	0.0399	0.4655	C_6	0.0411	0.3943	C_6	0.0456	0.4708	C_6	0.0286	0.3734	C_6	0.0761	0.4688	C_6	0.0489	0.2344
H_1	0.3441		H_1	0.3478		H_1	0.3491		H_1	0.3676		H_1	0.3508		H_1	0.3586	
H_2	0.1830	0.0133	C_2	-0.5428	-0.6601	H2	0.1867	0.0209	N_2	-1.0035	-0.8971	H_2	0.1836	0.0235	H_2	0.1491	0.0420
			H_{21}	0.2054	0.1555				H_{21}	0.4880	0.3602						
			H_{22}	0.1920	0.1792				H_{22}	0.4752	0.3683						
			H_{23}	0.1920	0.1792												
H_3	0.1801	0.1692	H_3	0.1851	0.1743	H	0.1903	0.1921	H_3	0.2084	0.1944	H_3	0.2096	0.2064	Cl_3	0.0558	-0.1026
H_4	0.1611	0.0819	H_4	0.1642	0.0914	C_4	-0.5446	-0.5163	H_4	0.1632	0.0953	N_4	-0.9612	-0.8774	H_4	0.1323	0.1244
						H_{31}	0.1877	0.1396				H_{41}	0.4677	0.3683			
						H_{32}	0.1875	0.1395				H_{42}	0.4677	0.3685			
						H_{33}	0.1950	0.1460									
H_5	0.1801	0.1693	H_5	0.1842	0.1662	H_5	0.1908	0.1923	H_5	0.1894	0.1670	H_5	0.2097	0.2059	H_5	0.1941	0.1256
H_6	0.1829	0.0131	H_6	0.1848	0.0332	H_6	0.1865	0.0209	H_6	0.1919	0.0416	H_6	0.1837	0.0237	H_6	0.1848	0.0667
																

Table S4f: Atomic partial charges, $\Delta G_{solv}(AH)$, $\Delta G_{solv}(A^-)$ and $\Delta\Delta G_{solv}$ for substituted imidazoles.

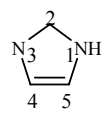
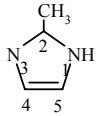
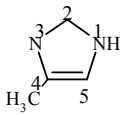
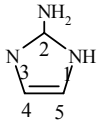
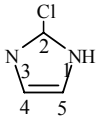
imidazole			2-methyl-imidazole			4-methyl-imidazole			2-amino-imidazole			2-chloro-imidazole		
	cation	neutral		Cation	neutral		cation	neutral		cation	Neutral		Cation	neutral
N_1	-0.1187	-0.2077	N_1	-0.1958	-0.2850	N_1	-0.1583	-0.2896	N_1	-0.2933	-0.3266	N_1	-0.0060	-0.1741
C_2	0.0345	0.2369	C_2	0.3793	0.5458	C_2	0.0304	0.2131	C_2	0.6505	0.7814	C_2	-0.0001	0.3210
N3	-0.1187	-0.5611	N3	-0.2083	-0.5898	N3	-0.2168	-0.5844	N3	-0.2930	-0.6306	N3	-0.0060	-0.4678
C_4	-0.1037	0.2104	C_4	-0.1253	0.1420	C_4	0.2588	0.4717	C_4	-0.1502	0.1291	C_4	-0.1382	0.1324
C_5	-0.1038	0.3421	C_5	-0.1348	-0.3550	C_5	-0.2037	-0.3616	C_5	-0.1502	-0.4125	C_5	-0.1383	-0.3145
H_1	0.3601	0.3021	H_1	0.3623	0.3184	H_1	0.3771	0.3330	H_1	0.3802	0.3311	H_1	0.3224	0.2933
H_2	0.2254	0.2020	C_2	-0.5441	-0.4886	H_2	0.2307	0.0977	N_2	-0.9855	-1.097	Cl_2	0.1684	-0.0945
			H_{21}	0.2029	0.1610				H_{21}	0.4859	0.4612			
			H_{22}	0.2101	0.1200				H_{22}	0.4860	0.4361			
			H_{23}	0.2134	0.1325									
H_3	0.3602		H_3	0.3674		H_3	0.3717		H_3	0.3800		H_3	0.3222	
H_4	0.2324	0.0746	H_4	0.2356	0.0916	C_4	-0.4711	-0.3977	H_4	0.2449	0.1064	H_4	0.2379	0.0991
						H_{41}	0.1709	0.1289						
						H_{42}	0.1852	0.0967						
						H_{43}	0.1852	0.0967						
H_5	0.2324	0.0847	H_5	0.2372	0.2070	H_5	0.2397	0.1953	H_5	0.2446	0.2218	H_5	0.2377	0.2052
														

Table S5: Complete list of gas phase quantities calculated with Becke($^1/_2$)/cc-pvqz on optimized geometries that were employed for the computations of pK_a values following equations 1-4, as explained in the text of the paper. The pK_a values depicted in Table 1 of the paper are base on these data.

gas phase energies for substituted carboxylic acids			
Substance	Energy terms	neutral	anion
propionic acid	E_0 (Hartrees)	-265.3341	-264.7728
	E_0 (kcal/mol)	-166499.8227	-166147.5672
	ZPVE (kcal/mol)	57.4470	48.5530
	EVE_{298} (kcal/mol)	-17.8803	-17.8792
	E_{gas}(298K) (kcal/mol)	-166460.2560	-166116.8934
	ΔE_{gas}(298K) (kcal/mol)	343.3627	
	PA (kcal/mol)	344.8427	
butyric acid	E_0 (Hartrees)	-304.08641	-303.52462
	E_0 (kcal/mol)	-190817.2605	-190464.7343
	ZPVE (kcal/mol)	75.6200	66.5750
	EVE_{298} (kcal/mol)	-19.2436	-19.1764
	E_{gas}(298K) (kcal/mol)	-190761.1058	-190417.3812
	ΔE_{gas}(298K) (kcal/mol)	343.5484	
	PA (kcal/mol)	345.0284	
2–chloropropionic acid	E_0 (Hartrees)	-723.19062	-722.64283
	E_0 (kcal/mol)	-453809.3446	-453465.5992
	ZPVE (kcal/mol)	51.922	43.05
	EVE_{298} (kcal/mol)	-19.9100	-19.1600
	E_{gas}(298K) (kcal/mol)	-453777.3326	-453441.7092
	ΔE_{gas}(298K) (kcal/mol)	335.6235	
	PA (kcal/mol)	337.1035	
3-chloropropionic acid	E_0 (Hartrees)	-723.19341	-722.64717
	E_0 (kcal/mol)	-453811.0966	-453468.3275
	ZPVE (kcal/mol)	52.303	43.389
	EVE_{298} (kcal/mol)	19.1022	19.0802
	E_{gas}(298K) (kcal/mol)	-453740.0824	-453406.1973
	ΔE_{gas}(298K) (kcal/mol)	333.8331	
	PA (kcal/mol)	335.3131	

gas phase energies for substituted benzoic acids

Substance	Energy terms	neutral	anion
benzoic acid	E_0 (Hartrees)	-415.85700	-415.30541
	E_0 (kcal/mol)	-260954.4261	-260608.2978
	ZPVE (kcal/mol)	73.8170	65.0620
	EVE_{298} (kcal/mol)	-19.8476	-19.7657
	E_{gas}(298K) (kcal/mol)	-260880.6091	-260543.2358
	ΔE_{gas}(298K) (kcal/mol)	337.3732	
	PA (kcal/mol)	338.9532	
p-methylbenzoic acid	E_0 (Hartrees)	-454.61283	-454.05908
	E_0 (kcal/mol)	-285274.0970	-284926.6133
	ZPVE (kcal/mol)	91.0610	82.2870
	EVE_{298} (kcal/mol)	-20.7581	-20.6706
	E_{gas}(298K) (kcal/mol)	-285203.794	-284864.9969
	ΔE_{gas}(298K) (kcal/mol)	338.7972	
	PA (kcal/mol)	340.2772	
m-methylbenzoic acid	E_0 (Hartrees)	-454.61166	-454.05885
	E_0 (kcal/mol)	-285273.3628	-284926.4690
	ZPVE (kcal/mol)	91.0880	82.3100
	EVE_{298} (kcal/mol)	-20.6935	-20.6091
	E_{gas}(298K) (kcal/mol)	-285202.9683	-284864.7681
	ΔE_{gas}(298K) (kcal/mol)	338.2002	
	PA (kcal/mol)	339.6802	
p-chlorobenzoic acid	E_0 (Hartrees)	-873.71706	-873.17224
	E_0 (kcal/mol)	-548266.1892	-547924.3106
	ZPVE (kcal/mol)	67.7800	59.0800
	EVE_{298} (kcal/mol)	-21.1646	-21.1009
	E_{gas}(298K) (kcal/mol)	-548198.4092	-547865.2306
	ΔE_{gas}(298K) (kcal/mol)	333.1786	
	PA (kcal/mol)	334.6586	

gas phase energies for substituted phenols			
substance	Energy terms	neutral	anion
phenol	E_0 (Hartrees)	-303.6690	-303.1029
	E_0 (kcal/mol)	-190555.3530	-190200.0757
	ZPVE (kcal/mol)	66.6750	57.5420
	EVE_{298} (kcal/mol)	-18.1397	-18.0639
	E_{gas}(298K) (kcal/mol)	-190506.8177	-190160.5976
	ΔE_{gas}(298K) (kcal/mol)	346.2201	
	PA (kcal/mol)	347.7001	
m-aminophenol	E_0 (Hartrees)	-358.4052	-357.8363
	E_0 (kcal/mol)	-224902.8533	-224545.8441
	ZPVE (kcal/mol)	77.2050	68.3610
	EVE_{298} (kcal/mol)	-19.2201	-19.2091
	E_{gas}(298K) (kcal/mol)	-224844.8684	-224496.6922
	ΔE_{gas}(298K) (kcal/mol)	348.18	
	PA (kcal/mol)	349.66	
o-aminophenol	E_0 (Hartrees)	-358.4021	-357.8353
	E_0 (kcal/mol)	-224900.8704	-224545.2228
	ZPVE (kcal/mol)	76.7000	67.9490
	EVE_{298} (kcal/mol)	-19.0016	-18.8047
	E_{gas}(298K) (kcal/mol)	-224843.1720	-224496.0785
	ΔE_{gas}(298K) (kcal/mol)	347.09	
	PA (kcal/mol)	348.57	
m-chlorophenol	E_0 (kcal/mol)	-761.5295	-760.9754
	ZPVE (kcal/mol)	-477867.3816	-477519.6864
	EVE_{298} (kcal/mol)	60.6940	51.6770
	E_{gas}(298K) (kcal/mol)	-19.5292	-19.4988
	E_{gas}(298K) (kcal/mol	-477827.1542	-477485.3901
	ΔE_{gas}(298K) (kcal/mol)	341.76	
	PA (kcal/mol)	343.24	
o-chlorophenol	E_0 (Hartrees)	-761.5314	-760.9724
	E_0 (kcal/mol)	-477868.5789	-477517.7606
	ZPVE (kcal/mol)	60.8660	51.8390
	EVE_{298} (kcal/mol)	-19.4413	-19.4685
	E_{gas}(298K) (kcal/mol)	-477827.1542	-477485.3901
	ΔE_{gas}(298K) (kcal/mol)	341.76	
	PA (kcal/mol)	343.24	

gas phase energies for substituted imides			
substance	energy terms	neutral	anion
glutarimide	E_0(Hartrees)	-395.34141	-394.77401
	E_0 (kcal/mol)	-248080.6882	-247724.64
	ZPVE (kcal/mol)	77.2450	68.2240
	EVE_{298} (kcal/mol)	-19.8700	-18.8944
	E_{gas}(298K) (kcal/mol)	-248023.3132	-247675.3094
	ΔE_{gas}(298K) (kcal/mol)	348.00	
	PA (kcal/mol)	349.48	
glutaconimide	E_0 (Hartrees)	-394.20021	-393.63578
	E_0 (kcal/mol)	-247364.5738	-247010.3883
	ZPVE (kcal/mol)	62.0650	53.0980
	EVE_{298} (kcal/mol)	-18.7901	-18.6752
	E_{gas}(298K) (kcal/mol)	-247321.2989	-246975.9655
	ΔE_{gas}(298K) (kcal/mol)	345.33	
	PA (kcal/mol)	346.81	

gas phase energies for substituted pyridines

substance	Energy terms	cation	neutral
pyridine	E_0 (Hartrees)	-245.4694	-245.1057
	E_0 (kcal/mol)	-154034.5258	-153806.2533
	ZPVE (kcal/mol)	65.3000	56.3680
	EVE_{298} (kcal/mol)	-17.2526	-17.1854
	E_{gas}(298K) (kcal/mol)	-153986.4784	-153767.0707
	ΔE_{gas}(298K) (kcal/mol)	219.4077	
	PA (kcal/mol)	220.8877	
2-methylpyridine	E_0 (Hartrees)	-284.2346	-283.8639
	E_0 (kcal/mol)	-178360.0407	-178127.4616
	ZPVE (kcal/mol)	82.5180	73.6150
	EVE_{298} (kcal/mol)	-18.1951	-18.1364
	E_{gas}(298K) (kcal/mol)	-178295.7178	-178071.9830
	ΔE_{gas}(298K) (kcal/mol)	223.7348	
	PA (kcal/mol)	225.2148	
4-methylpyridine	E_0 (Hartrees)	-284.2333	-283.8624
	E_0 (kcal/mol)	-178359.2318	-178126.4814
	ZPVE (kcal/mol)	82.4690	73.7050
	EVE_{298} (kcal/mol)	-18.2100	-18.1399
	E_{gas}(298K) (kcal/mol)	-178294.9728	-178070.9163
	ΔE_{gas}(298K) (kcal/mol)	224.0565	
	PA (kcal/mol)	225.5365	
2-aminopyridine	E_0 (Hartrees)	-300.2233	-299.8520
	E_0 (kcal/mol)	-188393.1424	-188160.1103
	ZPVE (kcal/mol)	75.5690	67.0610
	EVE_{298} (kcal/mol)	-18.4021	-18.2140
	E_{gas}(298K) (kcal/mol)	-188335.9755	-188111.2633
	ΔE_{gas}(298K) (kcal/mol)	224.7122	
	PA (kcal/mol)	226.1922	

4-aminopyridine	E_0 (Hartrees)	-300.2313	-299.8460
	E_0 (kcal/mol)	-188398.1443	-188156.3697
	ZPVE (kcal/mol)	76.1200	67.0460
	EVE_{298} (kcal/mol)	-18.2636	-18.2400
	E_{gas}(298K) (kcal/mol)	-188340.2879	-188107.5637
	ΔE_{gas}(298K) (kcal/mol)	232.7242	
	PA (kcal/mol)	234.2042	
3-chloropyridine	E_0 (Hartrees)	-703.3192	-702.9648
	E_0 (kcal/mol)	-441339.8017	-441117.4147
	ZPVE (kcal/mol)	59.2140	50.4280
	EVE_{298} (kcal/mol)	-18.6747	-18.6269
	E_{gas}(298K) (kcal/mol)	-441299.2624	-441085.6136
	ΔE_{gas}(298K) (kcal/mol)	213.6488	
	PA (kcal/mol)	215.1288	
	gas phase energies for substituted imidazoles		
substance	Energy terms	cation	neutral
Imidazole	E_0 (Hartrees)	-223.8254	-223.4561
	E_0 (kcal/mol)	-140452.6843	-140220.9235
	ZPVE (kcal/mol)	54.4150	45.4790
	EVE_{298} (kcal/mol)	-16.5269	-16.4954
	E_{gas}(298K) (kcal/mol)	-140414.7962	-140191.9399
	ΔE_{gas}(298K) (kcal/mol)	222.8563	
	PA (kcal/mol)	224.3363	
2-methylimidazole	E_0 (Hartrees)	-262.5936	-262.2157
	E_0 (kcal/mol)	-164780.0911	-164542.9777
	ZPVE (kcal/mol)	71.4840	62.6180
	EVE_{298} (kcal/mol)	-17.5223	-17.4906
	E_{gas}(298K) (kcal/mol)	-164726.1294	-164497.8503
	ΔE_{gas}(298K) (kcal/mol)	228.2791	
	PA (kcal/mol)	229.7591	
4-methylimidazole	E_0 (Hartrees)	-262.5876	-262.2124
	E_0 (kcal/mol)	-164776.3744	-164540.9069
	ZPVE (kcal/mol)	71.5900	62.6550
	EVE_{298} (kcal/mol)	-17.5292	-17.4898
	E_{gas}(298K) (kcal/mol)	-164722.3136	-164495.7417
	ΔE_{gas}(298K) (kcal/mol)	226.5719	
	PA (kcal/mol)	228.0519	

2-aminoimidazole	E_0 (Hartrees)	-278.5744	-278.1919
	E_0 (kcal/mol)	-174808.2299	-174568.1728
	ZPVE (kcal/mol)	63.9180	55.0460
	EVE_{298} (kcal/mol)	-18.0372	-17.6552
	E_{gas}(298K) (kcal/mol)	-174762.3491	-174530.7820
	ΔE_{gas}(298K) (kcal/mol)	231.5671	
	PA (kcal/mol)	233.0471	
2-chloroimidazole	E_0 (Hartrees)	-681.6733	-681.3137
	E_0 (kcal/mol)	-427756.7880	-427531.1555
	ZPVE (kcal/mol)	48.1200	39.4100
	EVE_{298} (kcal/mol)	-17.9987	-17.9775
	E_{gas}(298K) (kcal/mol)	-427726.6667	-427509.7230
	ΔE_{gas}(298K) (kcal/mol)	216.9437	
	PA (kcal/mol)	218.4237	

Table S6 : primary data for the 26 compounds included in our computation.

6 A.1.a.) primary data for propionic acid

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1       -0.0258522258      0.0047548982     -0.0284971816
H2       -0.5548701143     -0.8885542498     -0.3700288018
H3       -0.5852477203      0.8754526705     -0.3791707078
H4       -0.0368483611      0.0077087351      1.0652961329
C5        1.4136964851      0.0275375379     -0.5392499152
H6        1.9852308512     -0.8276699389     -0.1621371673
H7        1.9442436552      0.9150211462     -0.1724675641
C8        1.6010455091      0.0236892880     -2.0442825117
O9        0.4416877300      0.1736232881     -2.7316504415
O10       2.6713447798     -0.0885582605     -2.6007376844
H11       0.6913886354      0.1654238888     -3.6713507128
&
```

jaguar input to compute ZPVE and EVE^{298K}

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gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  carb   1      -0.0259   0.0048  -0.0285 -0.2072  2.000
ATOM      2  H2  carb   1      -0.5549  -0.8886  -0.3700  0.0672  1.200
ATOM      3  H3  carb   1      -0.5852   0.8755  -0.3792  0.0684  1.200
ATOM      4  H4  carb   1      -0.0368   0.0077   1.0653  0.0612  1.200
ATOM      5  C5  carb   1       1.4137   0.0275  -0.5392 -0.0131  2.000
ATOM      6  H6  carb   1       1.9852  -0.8277  -0.1621  0.0426  1.200
ATOM      7  H7  carb   1       1.9442   0.9150  -0.1725  0.0479  1.200
ATOM      8  C8  carb   1       1.6010   0.0237  -2.0443  0.6474  1.500
ATOM      9  O9  carb   1       0.4417   0.1736  -2.7317 -0.5832  1.400
ATOM     10  O10 carb   1       2.6713  -0.0886  -2.6007 -0.5608  1.400
ATOM     11  H11 carb   1       0.6914   0.1654  -3.6714  0.4294  1.000
```

6 A.1.b) primary data for propionic acid deprotonated (anion)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1       -0.0161789734     -0.0000552776     -0.0074516823
H2       -0.5465923608     -0.8962642862     -0.3473795159
H3       -0.5726588417      0.8527001239     -0.4076712679
H4       -0.0589745121      0.0305884015      1.0929625360
C5        1.4163274975      0.0125244384     -0.5425244875
H6        1.9783491199     -0.8575554999     -0.1735796295
H7        1.9578466940      0.8903361535     -0.1576333433
C8        1.5323352707      0.0350258484     -2.1154061661
O9        0.4487926275      0.1610393156     -2.7431554822
O10       2.7064366365     -0.0652585071     -2.5508321196
```

jaguar input to compute ZPVE and EVE^{298K}

```
gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  carb   1      -0.0162  -0.0001  -0.0075 -0.1748  2.000
ATOM      2  H2  carb   1      -0.5466  -0.8963  -0.3474  0.0304  1.200
ATOM      3  H3  carb   1      -0.5727   0.8527  -0.4077  0.0351  1.200
ATOM      4  H4  carb   1      -0.0590   0.0306   1.0930 -0.0182  1.200
ATOM      5  C5  carb   1       1.4163   0.0125  -0.5425  0.0247  2.000
ATOM      6  H6  carb   1       1.9783  -0.8576  -0.1736 -0.0375  1.200
ATOM      7  H7  carb   1       1.9578   0.8903  -0.1576 -0.0319  1.200
ATOM      8  C8  carb   1       1.5323   0.0350  -2.1154  0.6948  1.500
ATOM      9  O9  carb   1       0.4488   0.1610  -2.7432 -0.7449  1.400
ATOM     10  O10 carb   1       2.7064  -0.0653  -2.5508 -0.7775  1.400
```

6 A.2.a.) primary data for butyric acid

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1       -1.0941721436     -0.3214013191     -3.0012404172
H2       -0.9826296177     -1.1445934590     -3.7137328174
H3       -2.1658524727     -0.1719941992     -2.8285321674
H4       -0.7046413125      0.5859298791     -3.4758887806
C5       -0.3601495552     -0.6226839530     -1.6933868278
H6        0.7040411354     -0.7949833111     -1.8964436856
H7       -0.7485261542     -1.5441699554     -1.2465086759
C8       -0.4969333455      0.5251690567     -0.6734494194
H9       -0.0951490469      1.4555084753     -1.0826015738
H10      -1.5573046952      0.6794838479     -0.4399952597
C11       0.2434017646      0.2468288253      0.6142137757
O12       1.2275383664      0.8315493043      1.0106334516
O13      -0.3139315291     -0.7828753278      1.3044042507
H14       0.2392612626     -0.9006701163      2.0949287152
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  carb   1      -1.0942  -0.3214  -3.0012 -0.3340  2.000
ATOM      2  H2  carb   1      -0.9826  -1.1446  -3.7137  0.0838  1.200
ATOM      3  H3  carb   1      -2.1659  -0.1720  -2.8285  0.0832  1.200
ATOM      4  H4  carb   1      -0.7046   0.5859  -3.4759  0.0872  1.200
ATOM      5  C5  carb   1      -0.3601  -0.6227  -1.6934  0.1869  2.000
ATOM      6  H6  carb   1       0.7040  -0.7950  -1.8964 -0.0050  1.200
ATOM      7  H7  carb   1      -0.7485  -1.5442  -1.2465 -0.0037  1.200
ATOM      8  C8  carb   1      -0.4969   0.5252  -0.6734 -0.1687  2.000
ATOM      9  H9  carb   1      -0.0951   1.4555  -1.0826  0.0550  1.200
ATOM     10  H10 carb   1      -1.5573   0.6795  -0.4400  0.0817  1.200
ATOM     11  C11 carb   1       0.2434   0.2468   0.6142  0.6158  1.500
ATOM     12  O12 carb   1       1.2275   0.8315   1.0106 -0.5247  1.400
ATOM     13  O13 carb   1      -0.3139  -0.7829   1.3044 -0.5835  1.400
ATOM     14  H14 carb   1       0.2393  -0.9007   2.0949  0.4256  1.000
```

6 A.2.b.) primary data for butyric acid deprotonated (anion)

jaguar input to estimate the electronic energy of butyric acid deprotonated (anion)

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1       -1.1382153686     -0.3512700080     -3.0155370379
H2       -1.1169143774     -1.2119238352     -3.6994088810
H3       -2.1909501682     -0.1386613986     -2.7866551489
H4       -0.7493262727      0.5155119396     -3.5669111480
C5       -0.3379116067     -0.6096662165     -1.7301227957
H6        0.6992657464     -0.8615664745     -1.9962497233
H7       -0.7254453145     -1.4823492734     -1.1933373270
C8       -0.3391614902      0.5511210137     -0.7343935263
H9        0.2141900145      1.4170699041     -1.1225512176
H10      -1.3774611173      0.8946472942     -0.5881100097
C11       0.2282523510      0.1724491326      0.6912792735
O12       0.7197146005      1.1284479661      1.3387637824
O13       0.0866450489     -1.0343337762      1.0237604606
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  carb   1      -1.1382  -0.3513  -3.0155 -0.2957  2.000
ATOM      2  H2  carb   1      -1.1169  -1.2119  -3.6994  0.0322  1.200
ATOM      3  H3  carb   1      -2.1910  -0.1387  -2.7867  0.0498  1.200
ATOM      4  H4  carb   1      -0.7493   0.5155  -3.5669  0.0435  1.200
ATOM      5  C5  carb   1      -0.3379  -0.6097  -1.7301  0.2116  2.000
ATOM      6  H6  carb   1       0.6993  -0.8616  -1.9962 -0.0483  1.200
ATOM      7  H7  carb   1      -0.7254  -1.4823  -1.1933 -0.0287  1.200
ATOM      8  C8  carb   1      -0.3392   0.5511  -0.7344 -0.1490  2.000
ATOM      9  H9  carb   1       0.2142   1.4171  -1.1226 -0.0159  1.200
ATOM     10  H10 carb   1      -1.3775   0.8946  -0.5881  0.0095  1.200
ATOM     11  C11 carb   1       0.2283   0.1724   0.6913  0.6931  1.500
ATOM     12  O12 carb   1       0.7197   1.1284   1.3388 -0.7554  1.400
ATOM     13  O13 carb   1       0.0866  -1.0343   1.0238 -0.7465  1.400
```

6 A.3.a.) primary data for 2-chloropropionic acid

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1       -0.1982332417     -0.6930671295     -1.7689424294
H2        0.8550581314     -0.9063812409     -1.9823976640
H3       -0.6935278881     -0.4215317679     -2.7035355038
H4       -0.6659854380     -1.5923541625     -1.3641444756
C5       -0.2892565094      0.4574424418     -0.7726436976
H6        0.1593014043      1.3688773340     -1.1656783130
Cl       -2.0350344732      0.8739674893     -0.4380035974
C8        0.4259071221      0.1545464216      0.5377023217
O9        1.3872873528      0.7739613943      0.9318579601
O10      -0.0920339984     -0.9088893305      1.1831774787
H11       0.4383964463     -1.0228370838      1.9897987638
&
&atomic
atom    basis
Cl      6-31g**
```

jaguar input to compute ZPVE and EVE^{298K}

```
gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  carb   1      -0.1982  -0.6931  -1.7689 -0.2389  2.000
ATOM      2  H2  carb   1       0.8551  -0.9064  -1.9824  0.1006  1.200
ATOM      3  H3  carb   1      -0.6935  -0.4215  -2.7035  0.0971  1.200
ATOM      4  H4  carb   1      -0.6660  -1.5924  -1.3641  0.1029  1.200
ATOM      5  C5  carb   1      -0.2893   0.4574  -0.7726 -0.0169  2.000
ATOM      6  H6  carb   1       0.1593   1.3689  -1.1657  0.1148  1.200
ATOM      7  Cl  carb   1      -2.0350   0.8740  -0.4380 -0.1635  1.900
ATOM      8  C8  carb   1       0.4259   0.1545   0.5377  0.6351  1.500
ATOM      9  O9  carb   1       1.3873   0.7740   0.9319 -0.5095  1.400
ATOM     10  O10 carb   1      -0.0920  -0.9089   1.1832 -0.5540  1.400
ATOM     11  H11 carb   1       0.4384  -1.0228   1.9898  0.4321  1.000
```

6 A.3.b.) primary data for 2-chloropropionic acid deprotonated (anion)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1       -0.3702546652     -0.8077881332     -1.6572920019
H2        0.5710338878     -1.3598366501     -1.7044525658
H3       -0.6741168328     -0.4905406871     -2.6622230686
H4       -1.1281732644     -1.4880124454     -1.2574263886
C5       -0.1599654575      0.3693170746     -0.7182754125
H6        0.5229775966      1.0985589807     -1.1671835438
Cl       -1.7609072508      1.3305729037     -0.6232558664
C8        0.4228616141     -0.0193180562      0.7113824404
O9        0.2931766910      0.8176615290      1.6211514220
O10       1.0195258678     -1.1242518440      0.6797203831
&
&atomic
atom    basis
Cl      6-31g**
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  carb   1      -0.3703  -0.8078  -1.6573 -0.2619  2.000
ATOM      2  H2  carb   1       0.5710  -1.3598  -1.7045  0.0780  1.200
ATOM      3  H3  carb   1      -0.6741  -0.4905  -2.6622  0.0259  1.200
ATOM      4  H4  carb   1      -1.1282  -1.4880  -1.2574  0.0759  1.200
ATOM      5  C5  carb   1      -0.1600   0.3693  -0.7183  0.1391  2.000
ATOM      6  H6  carb   1       0.5230   1.0986  -1.1672  0.0359  1.200
ATOM      7  Cl  carb   1      -1.7609   1.3306  -0.6233 -0.3450  1.900
ATOM      8  C8  carb   1       0.4229  -0.0193   0.7114  0.7025  1.500
ATOM      9  O9  carb   1       0.2932   0.8177   1.6212 -0.7270  1.400
ATOM     10  O10 carb   1       1.0195  -1.1243   0.6797 -0.7235  1.400
```

6 A.4.a.) primary data for 3-chloropropionic acid

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1       -0.0119333465     -0.0017177359     -0.2931262997
H2       -0.5214767122     -0.9068988314     -0.6231424840
H3       -0.5697100508      0.8647548765     -0.6456631443
Cl       -0.1062443867      0.0155458549      1.5202974854
C5        1.4408527336      0.0323459496     -0.7493863184
H6        1.9993991466     -0.8158708480     -0.3430846486
H7        1.9379543247      0.9324577832     -0.3702349482
C8        1.6409409831      0.0164327701     -2.2552177055
O9        0.4884908969      0.2078938737     -2.9432716718
O10       2.7095687027     -0.1348577154     -2.7993150294
H11       0.7288917277      0.1904278998     -3.8856985671
&
&atomic
atom    basis
Cl     6-31g**
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  carb   1      -0.0119  -0.0017  -0.2931 -0.1621  2.000
ATOM      2  H2  carb   1      -0.5215  -0.9069  -0.6231  0.1388  1.200
ATOM      3  H3  carb   1      -0.5697   0.8648  -0.6457  0.1424  1.200
ATOM      4  Cl  carb   1      -0.1062   0.0155   1.5203 -0.1785  1.900
ATOM      5  C5  carb   1       1.4409   0.0323  -0.7494 -0.0536  2.000
ATOM      6  H6  carb   1       1.9994  -0.8159  -0.3431  0.0696  1.200
ATOM      7  H7  carb   1       1.9380   0.9325  -0.3702  0.0767  1.200
ATOM      8  C8  carb   1       1.6409   0.0164  -2.2552  0.6804  1.500
ATOM      9  O9  carb   1       0.4885   0.2079  -2.9433 -0.6059  1.400
ATOM     10  O10 carb   1       2.7096  -0.1349  -2.7993 -0.5486  1.400
ATOM     11  H11 carb   1       0.7289   0.1904  -3.8857  0.4407  1.000
```

6 A.4.b.) primary data for 3-chloropropionic acid deprotonated (anion)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1       0.0477091338     -0.0116086448     -0.3198226721
H2      -0.4688838220     -0.9200923624     -0.6228601683
H3      -0.4991957626      0.8492519372     -0.6945511101
Cl      -0.1813296933      0.0451673207      1.5558028860
C5       1.4933531039      0.0067240896     -0.7426093813
H6       2.0330386627     -0.8653950084     -0.3576397920
H7       2.0003964545      0.8947156738     -0.3461577729
C8       1.5965176912      0.0288298614     -2.3290545631
O9       0.4978113285      0.1749256620     -2.9257426694
O10      2.7553935729     -0.0914134329     -2.7764674052
&
&atomic
atom    basis
Cl      6-31g**
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  carb   1       0.0477  -0.0116  -0.3198  0.0164  2.000
ATOM      2  H2  carb   1      -0.4689  -0.9201  -0.6229  0.0790  1.200
ATOM      3  H3  carb   1      -0.4992   0.8493  -0.6946  0.0860  1.200
ATOM      4  Cl  carb   1      -0.1813   0.0452   1.5558 -0.3561  1.900
ATOM      5  C5  carb   1       1.4934   0.0067  -0.7426 -0.0719  2.000
ATOM      6  H6  carb   1       2.0330  -0.8654  -0.3576  0.0086  1.200
ATOM      7  H7  carb   1       2.0004   0.8947  -0.3462  0.0165  1.200
ATOM      8  C8  carb   1       1.5965   0.0288  -2.3291  0.7120  1.500
ATOM      9  O9  carb   1       0.4978   0.1749  -2.9257 -0.7443  1.400
ATOM     10  O10 carb   1       2.7554  -0.0914  -2.7765 -0.7463  1.400
```

6 B.1.a) primary data for benzoic acid

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1        1.2353008739      0.5050530482      0.0000000000
C2        1.2540242731      1.8974192353      0.0000000000
C3        0.0516194985      2.6115261292      0.0000000000
C4       -1.1693528922      1.9315098724      0.0000000000
C5       -1.1927539850      0.5377267322      0.0000000000
C6        0.0116812124     -0.1791084223      0.0000000000
H7        2.1537078399     -0.0724730228      0.0000000000
H8        2.2017358975      2.4276139420      0.0000000000
H9        0.0668956900      3.6978375955      0.0000000000
H10      -2.1021877762      2.4873313657      0.0000000000
H11      -2.1350598177      0.0014977530      0.0000000000
C12       0.0476235596     -1.6653852055      0.0000000000
O13       1.0610625776     -2.3365072714      0.0000000000
O14      -1.1863634025     -2.2310937244      0.0000000000
H15      -1.0319992424     -3.1901929088      0.0000000000
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  benz   1       1.2353   0.5051   0.0000  -0.1392  1.500
ATOM      2  C2  benz   1       1.2540   1.8974   0.0000  -0.1104  1.500
ATOM      3  C3  benz   1       0.0516   2.6115   0.0000  -0.0983  1.500
ATOM      4  C4  benz   1      -1.1694   1.9315   0.0000  -0.1194  1.500
ATOM      5  C5  benz   1      -1.1928   0.5377   0.0000  -0.1342  1.500
ATOM      6  C6  benz   1       0.0117  -0.1791   0.0000   0.0175  1.500
ATOM      7  H7  benz   1       2.1537  -0.0725   0.0000   0.1383  1.200
ATOM      8  H8  benz   1       2.2017   2.4276   0.0000   0.1224  1.200
ATOM      9  H9  benz   1       0.0669   3.6978   0.0000   0.1212  1.200
ATOM     10  H10 benz   1      -2.1022   2.4873   0.0000   0.1229  1.200
ATOM     11  H11 benz   1      -2.1351   0.0015   0.0000   0.1412  1.200
ATOM     12  C12 benz   1       0.0476  -1.6654   0.0000   0.6086  1.500
ATOM     13  O13 benz   1       1.0611  -2.3365   0.0000  -0.5252  1.400
ATOM     14  O14 benz   1      -1.1864  -2.2311   0.0000  -0.5748  1.400
ATOM     15  H15 benz   1      -1.0320  -3.1902   0.0000   0.4290  1.000
```

6 B.1.b) primary data for benzoic acid deprotonated (anion)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1        1.2139243925      0.4737270323      0.0000000000
C2        1.2556492433      1.8692152123      0.0000000000
C3        0.0664208103      2.6064896392      0.0000000000
C4       -1.1594516876      1.9327325930      0.0000000000
C5       -1.1904232246      0.5362500550      0.0000000000
C6       -0.0073977108     -0.2125598684      0.0000000000
H7        2.1128744665     -0.1370348546      0.0000000000
H8        2.2128214101      2.3906380463      0.0000000000
H9        0.0965554073      3.6952164761      0.0000000000
H10      -2.0885681579      2.5021671086      0.0000000000
H11      -2.1226710218     -0.0219474490      0.0000000000
C12      -0.0448275809     -1.7718254194      0.0000000000
O13       1.0811706402     -2.3297515061      0.0000000000
O14      -1.1949189302     -2.2781722932      0.0000000000
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  benz   1       1.2139   0.4737   0.0000  -0.1318  1.500
ATOM      2  C2  benz   1       1.2556   1.8692   0.0000  -0.1444  1.500
ATOM      3  C3  benz   1       0.0664   2.6065   0.0000  -0.1528  1.500
ATOM      4  C4  benz   1      -1.1595   1.9327   0.0000  -0.1444  1.500
ATOM      5  C5  benz   1      -1.1904   0.5363   0.0000  -0.1324  1.500
ATOM      6  C6  benz   1      -0.0074  -0.2126   0.0000   0.0171  1.500
ATOM      7  H7  benz   1       2.1129  -0.1370   0.0000   0.1022  1.200
ATOM      8  H8  benz   1       2.2128   2.3906   0.0000   0.0857  1.200
ATOM      9  H9  benz   1       0.0966   3.6952   0.0000   0.0895  1.200
ATOM     10  H10 benz   1      -2.0886   2.5022   0.0000   0.0860  1.200
ATOM     11  H11 benz   1      -2.1227  -0.0219   0.0000   0.1020  1.200
ATOM     12  C12 benz   1      -0.0448  -1.7718   0.0000   0.6503  1.500
ATOM     13  O13 benz   1       1.0812  -2.3298   0.0000  -0.7133  1.400
ATOM     14  O14 benz   1      -1.1949  -2.2782   0.0000  -0.7136  1.400
```

6 B.2.a) primary data for m-methylbenzoic acid

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1        0.9477149385      0.2370770997      0.0000000000
C2        0.9792581356      1.6353785993      0.0000000000
C3       -0.2412892183      2.3244830058      0.0000000000
C4       -1.4594289866      1.6392825291      0.0000000000
C5       -1.4807321619      0.2474169812      0.0000000000
C6       -0.2678439912     -0.4562413374      0.0000000000
H7        1.8684600497     -0.3390922906      0.0000000000
H8       -0.2369968373      3.4118197378      0.0000000000
H9       -2.3919280524      2.1957724083      0.0000000000
H10      -2.4191543575     -0.2949003311      0.0000000000
C11      -0.2155597350     -1.9420242642      0.0000000000
O12      -1.4434641673     -2.5211745142      0.0000000000
O13       0.8044091597     -2.6036903210      0.0000000000
H14      -1.2779739485     -3.4784133333      0.0000000000
C15       2.2972652445      2.3740115131      0.0000000000
```

```
H16       2.8957969200                  2.1175219668      0.8812174607
H17       2.1477738875      3.4570451235      0.0000000000
H18       2.8957969200      2.1175219668     -0.8812174607
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  benz   1       0.9477   0.2371   0.0000  -0.2724  1.500
ATOM      2  C2  benz   1       0.9793   1.6354   0.0000   0.2787  1.500
ATOM      3  C3  benz   1      -0.2413   2.3245   0.0000  -0.2316  1.500
ATOM      4  C4  benz   1      -1.4594   1.6393   0.0000  -0.1044  1.500
ATOM      5  C5  benz   1      -1.4807   0.2474   0.0000  -0.1742  1.500
ATOM      6  C6  benz   1      -0.2678  -0.4562   0.0000   0.0207  1.500
ATOM      7  H7  benz   1       1.8685  -0.3391   0.0000   0.1644  1.200
ATOM      8  H8  benz   1      -0.2370   3.4118   0.0000   0.1458  1.200
ATOM      9  H9  benz   1      -2.3919   2.1958   0.0000   0.1296  1.200
ATOM     10  H10 benz   1      -2.4192  -0.2949   0.0000   0.1504  1.200
ATOM     11  C11 benz   1      -0.2156  -1.9420   0.0000   0.6377  1.500
ATOM     12  O12 benz   1      -1.4435  -2.5212   0.0000  -0.5813  1.400
ATOM     13  O13 benz   1       0.8044  -2.6037   0.0000  -0.5314  1.400
ATOM     14  H14 benz   1      -1.2780  -3.4784   0.0000   0.4275  1.000
ATOM     15  C15 benz   1       2.2973   2.3740   0.0000  -0.4449  2.000
ATOM     16  H16 benz   1       2.8958   2.1175   0.8812   0.1319  1.200
ATOM     17  H17 benz   1       2.1478   3.4570   0.0000   0.1214  1.200
ATOM     18  H18 benz   1       2.8958   2.1175  -0.8812   0.1319  1.200
```

6 B.2.b) primary data for m-methylbenzoic acid deprotonated (anion)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1         0.9237662272      0.2097379428      0.0000000000
C2         0.9713104262      1.6101779638      0.0000000000
C3        -0.2349922978      2.3220568346      0.0000000000
C4        -1.4569340792      1.6401660468      0.0000000000
C5        -1.4809636810      0.2460862437      0.0000000000
C6        -0.2873029628     -0.4883370908      0.0000000000
H7         1.8273041207     -0.3969049174      0.0000000000
H8        -0.2158571412      3.4118842638      0.0000000000
H9        -2.3871814089      2.2075154248      0.0000000000
H10       -2.4078128057     -0.3203971346      0.0000000000
C11       -0.3058801643     -2.0481093349      0.0000000000
O12       -1.4501275972     -2.5677353847      0.0000000000
O13        0.8267145405     -2.5933806495      0.0000000000
C14        2.3000348427      2.3386272915      0.0000000000
H15        2.9028017032      2.0803084083      0.8800753983
H16        2.1634757726      3.4262981733      0.0000000000
H17        2.9028017032      2.0803084083     -0.8800753983
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  benz   1       0.9238   0.2097   0.0000  -0.2846  1.500
ATOM      2  C2  benz   1       0.9713   1.6102   0.0000   0.2584  1.500
ATOM      3  C3  benz   1      -0.2350   2.3221   0.0000  -0.3067  1.500
ATOM      4  C4  benz   1      -1.4569   1.6402   0.0000  -0.1163  1.500
ATOM      5  C5  benz   1      -1.4810   0.2461   0.0000  -0.1810  1.500
ATOM      6  C6  benz   1      -0.2873  -0.4883   0.0000   0.0419  1.500
ATOM      7  H7  benz   1       1.8273  -0.3969   0.0000   0.1375  1.200
ATOM      8  H8  benz   1      -0.2159   3.4119   0.0000   0.1218  1.200
ATOM      9  H9  benz   1      -2.3872   2.2075   0.0000   0.0911  1.200
ATOM     10  H10 benz   1      -2.4078  -0.3204   0.0000   0.1136  1.200
ATOM     11  C11 benz   1      -0.3059  -2.0481   0.0000   0.6714  1.500
ATOM     12  O12 benz   1      -1.4501  -2.5677   0.0000  -0.7174  1.400
ATOM     13  O13 benz   1       0.8267  -2.5934   0.0000  -0.7190  1.400
ATOM     14  C14 benz   1       2.3000   2.3386   0.0000  -0.3875  2.000
ATOM     15  H15 benz   1       2.9028   2.0803   0.8801   0.0975  1.200
ATOM     16  H16 benz   1       2.1635   3.4263   0.0000   0.0816  1.200
ATOM     17  H17 benz   1       2.9028   2.0803  -0.8801   0.0975  1.200
```

6 B.3.a) primary data for p-methylbenzoic acid

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1        1.2236945792      0.0708080418      0.0000000000
C2        1.2360142973      1.4598370186      0.0000000000
C3        0.0366937507      2.1925645799      0.0000000000
C4       -1.1748162081      1.4888968957      0.0000000000
C5       -1.1973084479      0.0954750665      0.0000000000
C6        0.0041518950     -0.6228787468      0.0000000000
H7        2.1467565747     -0.4994047244      0.0000000000
H8        2.1853751365      1.9898505723      0.0000000000
H9       -2.1116881512      2.0396821830      0.0000000000
H10      -2.1415681287     -0.4373901297      0.0000000000
C11       0.0437523817     -2.1060782399      0.0000000000
O12      -1.1894231748     -2.6756358943      0.0000000000
O13       1.0581934248     -2.7766538663      0.0000000000
H14      -1.0307936776     -3.6339405372      0.0000000000
C15       0.0633013176      3.7015795703      0.0000000000
H16      -0.9462610516      4.1206026561      0.0000000000
H17       0.5885140949      4.0875398905      0.8811163962
H18       0.5885140949      4.0875398905     -0.8811163962
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  benz   1       1.2237   0.0708   0.0000  -0.1232  1.500
ATOM      2  C2  benz   1       1.2360   1.4598   0.0000  -0.2366  1.500
ATOM      3  C3  benz   1       0.0367   2.1926   0.0000   0.2949  1.500
ATOM      4  C4  benz   1      -1.1748   1.4889   0.0000  -0.2559  1.500
ATOM      5  C5  benz   1      -1.1973   0.0955   0.0000  -0.1087  1.500
ATOM      6  C6  benz   1       0.0042  -0.6229   0.0000  -0.0370  1.500
ATOM      7  H7  benz   1       2.1468  -0.4994   0.0000   0.1458  1.200
ATOM      8  H8  benz   1       2.1854   1.9899   0.0000   0.1437  1.200
ATOM      9  H9  benz   1      -2.1117   2.0397   0.0000   0.1444  1.200
ATOM     10  H10 benz   1      -2.1416  -0.4374   0.0000   0.1478  1.200
ATOM     11  C11 benz   1       0.0438  -2.1061   0.0000   0.6370  1.500
ATOM     12  O12 benz   1      -1.1894  -2.6756   0.0000  -0.5833  1.400
ATOM     13  O13 benz   1       1.0582  -2.7767   0.0000  -0.5408  1.400
ATOM     14  H14 benz   1      -1.0308  -3.6339   0.0000   0.4270  1.000
ATOM     15  C15 benz   1       0.0633   3.7016   0.0000  -0.4478  2.000
ATOM     16  H16 benz   1      -0.9463   4.1206   0.0000   0.1276  1.200
ATOM     17  H17 benz   1       0.5885   4.0875   0.8811   0.1326  1.200
ATOM     18  H18 benz   1       0.5885   4.0875  -0.8811   0.1326  1.200
```

6 B.3.b) primary data for p-methylbenzoic acid deprotonated (anion)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1        1.1980169825      0.0393843425      0.0000000000
C2        1.2302401631      1.4322239335      0.0000000000
C3        0.0421337810      2.1809659224      0.0000000000
C4       -1.1729431331      1.4842368183      0.0000000000
C5       -1.2001452805      0.0872753563      0.0000000000
C6       -0.0178944942     -0.6582912003      0.0000000000
H7        2.1026091970     -0.5630291192      0.0000000000
H8        2.1871090015      1.9569334976      0.0000000000
H9       -2.1064555597      2.0483880650      0.0000000000
H10      -2.1328718992     -0.4701091985      0.0000000000
C11      -0.0454506169     -2.2163501935      0.0000000000
O12      -1.1921840371     -2.7300756805      0.0000000000
O13       1.0847146205     -2.7666139510      0.0000000000
C14       0.0814942400      3.6943820007      0.0000000000
H15      -0.9283809733      4.1191452827      0.0000000000
H16       0.6044724713      4.0911561721      0.8807123348
H17       0.6044724713      4.0911561721     -0.8807123348
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  benz   1       1.1980   0.0394   0.0000  -0.1112  1.500
ATOM      2  C2  benz   1       1.2302   1.4322   0.0000  -0.2830  1.500
ATOM      3  C3  benz   1       0.0421   2.1810   0.0000   0.2379  1.500
ATOM      4  C4  benz   1      -1.1729   1.4842   0.0000  -0.2887  1.500
ATOM      5  C5  benz   1      -1.2001   0.0873   0.0000  -0.1129  1.500
ATOM      6  C6  benz   1      -0.0179  -0.6583   0.0000  -0.0229  1.500
ATOM      7  H7  benz   1       2.1026  -0.5630   0.0000   0.1099  1.200
ATOM      8  H8  benz   1       2.1871   1.9569   0.0000   0.1162  1.200
ATOM      9  H9  benz   1      -2.1065   2.0484   0.0000   0.1168  1.200
ATOM     10  H10 benz   1      -2.1329  -0.4701   0.0000   0.1104  1.200
ATOM     11  C11 benz   1      -0.0455  -2.2164   0.0000   0.6752  1.500
ATOM     12  O12 benz   1      -1.1922  -2.7301   0.0000  -0.7195  1.400
ATOM     13  O13 benz   1       1.0847  -2.7666   0.0000  -0.7186  1.400
ATOM     14  C14 benz   1       0.0815   3.6944   0.0000  -0.3796  2.000
ATOM     15  H15 benz   1      -0.9284   4.1191   0.0000   0.0898  1.200
ATOM     16  H16 benz   1       0.6045   4.0912   0.8807   0.0902  1.200
ATOM     17  H17 benz   1       0.6045   4.0912  -0.8807   0.0902  1.200
```

6 B.4.a) primary data for p-chlorobenzoic acid

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1         1.2161563867      0.4443710320      0.0000000000
C2         1.2443943821     -0.9462594068      0.0000000000
C3         0.0359082402     -1.6474046980      0.0000000000
C4        -1.1913619852     -0.9810049151      0.0000000000
C5        -1.2075483391      0.4113569007      0.0000000000
C6        -0.0052944155      1.1312530128      0.0000000000
H7         2.1373959821      1.0171290797      0.0000000000
H8         2.1856284880     -1.4841811520      0.0000000000
Cl         0.0595606836     -3.4008835072      0.0000000000
H10       -2.1162912511     -1.5465104861      0.0000000000
H11       -2.1525002041      0.9422750269      0.0000000000
C12        0.0316625387      2.6179504691      0.0000000000
O13        1.0439523336      3.2882455303      0.0000000000
O14       -1.2039973175      3.1805787981      0.0000000000
H15       -1.0562567606      4.1408211938      0.0000000000
&
&atomic
atom    basis
Cl      6-31g**
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  benz   1       1.2162   0.4444   0.0000 -0.1742  1.500
ATOM      2  C2  benz   1       1.2444  -0.9463   0.0000 -0.0466  1.500
ATOM      3  C3  benz   1       0.0359  -1.6474   0.0000  0.0335  1.500
ATOM      4  C4  benz   1      -1.1914  -0.9810   0.0000 -0.0565  1.500
ATOM      5  C5  benz   1      -1.2075   0.4114   0.0000 -0.1680  1.500
ATOM      6  C6  benz   1      -0.0053   1.1313   0.0000  0.0129  1.500
ATOM      7  H7  benz   1       2.1374   1.0171   0.0000  0.1570  1.200
ATOM      8  H8  benz   1       2.1856  -1.4842   0.0000  0.1157  1.200
ATOM      9  Cl  benz   1       0.0596  -3.4009   0.0000 -0.0955  1.900
ATOM     10  H10 benz   1      -2.1163  -1.5465   0.0000  0.1160  1.200
ATOM     11  H11 benz   1      -2.1525   0.9423   0.0000  0.1602  1.200
ATOM     12  C12 benz   1       0.0317   2.6180   0.0000  0.6218  1.500
ATOM     13  O13 benz   1       1.0440   3.2882   0.0000 -0.5292  1.400
ATOM     14  O14 benz   1      -1.2040   3.1806   0.0000 -0.5770  1.400
ATOM     15  H15 benz   1      -1.0563   4.1408   0.0000  0.4297  1.000
```

6 B.4.b) primary data for p- chlorobenzoic acid deprotonated (anion)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1         1.1899376942     -0.4864406887      0.0000000000
C2         1.2415025641      0.9094352920      0.0000000000
C3         0.0417899880      1.6205032891      0.0000000000
C4        -1.1927566632      0.9715138708      0.0000000000
C5        -1.2130042970     -0.4250350718      0.0000000000
C6        -0.0297591003     -1.1719074170      0.0000000000
H7         2.0941092996     -1.0886626927      0.0000000000
H8         2.1885083755      1.4418566216      0.0000000000
Cl         0.0867597868      3.4020709685      0.0000000000
H10       -2.1109785443      1.5522119904      0.0000000000
H11       -2.1456176533     -0.9822199741      0.0000000000
C12       -0.0696752771     -2.7304355903      0.0000000000
O13        1.0559341825     -3.2853686773      0.0000000000
O14       -1.2232707560     -3.2259841603      0.0000000000
&
&atomic
atom    basis
Cl      6-31g**
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ip172=2
basis=6-31g**
```

```
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  benz   1       1.1899  -0.4864   0.0000  -0.1540  1.500
ATOM      2  C2  benz   1       1.2415   0.9094   0.0000  -0.1286  1.500
ATOM      3  C3  benz   1       0.0418   1.6205   0.0000   0.0827  1.500
ATOM      4  C4  benz   1      -1.1928   0.9715   0.0000  -0.1284  1.500
ATOM      5  C5  benz   1      -1.2130  -0.4250   0.0000  -0.1539  1.500
ATOM      6  C6  benz   1      -0.0298  -1.1719   0.0000   0.0025  1.500
ATOM      7  H7  benz   1       2.0941  -1.0887   0.0000   0.1247  1.200
ATOM      8  H8  benz   1       2.1885   1.4419   0.0000   0.0996  1.200
ATOM      9  Cl  benz   1       0.0868   3.4021   0.0000  -0.2023  1.900
ATOM     10  H10 benz   1      -2.1110   1.5522   0.0000   0.0995  1.200
ATOM     11  H11 benz   1      -2.1456  -0.9822   0.0000   0.1248  1.200
ATOM     12  C12 benz   1      -0.0697  -2.7304   0.0000   0.6694  1.500
ATOM     13  O13 benz   1       1.0559  -3.2854   0.0000  -0.7178  1.400
ATOM     14  O14 benz   1      -1.2233  -3.2260   0.0000  -0.7182  1.400
```

6 C.1.a) primary data for phenol

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C       1.1618973542      0.4114092132      0.0000000000
C       0.4573681942     -0.7977258447      0.0000000000
C      -0.9411851283     -0.7952099629      0.0000000000
C      -1.6257912505      0.4184276118      0.0000000000
C      -0.9313662993      1.6317453634      0.0000000000
C       0.4647486191      1.6198156472      0.0000000000
O       1.0827751037     -2.0138259271      0.0000000000
H       2.0385691229     -1.8739439480      0.0000000000
H       2.2503572176      0.4056065196      0.0000000000
H       1.0179751950      2.5547485103      0.0000000000
H      -1.4679286570     -1.7437802690      0.0000000000
H      -2.7122640633      0.4149503127      0.0000000000
H      -1.4709681869      2.5736066864      0.0000000000
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
```

```
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  phen   1       1.2176  -0.1968   0.0000  -0.3324  1.500
ATOM      2  C2  phen   1       1.1846   1.1990   0.0000  -0.0490  1.500
ATOM      3  C3  phen   1      -0.0339   1.8791   0.0000  -0.1869  1.500
ATOM      4  C4  phen   1      -1.2265   1.1470   0.0000  -0.0889  1.500
ATOM      5  C5  phen   1      -1.2070  -0.2456   0.0000  -0.2479  1.500
ATOM      6  C6  phen   1       0.0197  -0.9193   0.0000   0.3999  1.500
ATOM      7  H7  phen   1       2.1700  -0.7255   0.0000   0.1472  1.200
ATOM      8  H8  phen   1       2.1201   1.7526   0.0000   0.1169  1.200
ATOM      9  H9  phen   1      -2.1823   1.6648   0.0000   0.1211  1.200
ATOM     10  H10 phen   1      -2.1242  -0.8268   0.0000   0.1601  1.200
ATOM     11  H11 phen   1      -0.0560   2.9650   0.0000   0.1230  1.200
ATOM     12  O12 phen   1      -0.0175  -2.2871   0.0000  -0.5717  1.400
ATOM     13  H13 phen   1       0.8909  -2.6260   0.0000   0.4086  1.000
```

6 C.1.b) primary data for phenoxide

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1        1.2132839246      1.1385768968      0.0000000000
C2        1.2112653367     -0.2497342630      0.0000000000
C3       -0.0105832037     -1.0358913189      0.0000000000
C4       -1.2165505152     -0.2271565199      0.0000000000
C5       -1.1907996742      1.1616417620      0.0000000000
C6        0.0176160224      1.8794869515      0.0000000000
O7       -0.0209131986     -2.3018664304      0.0000000000
H8        2.1482639511     -0.8068557048      0.0000000000
H9        2.1685172833      1.6701613939      0.0000000000
H10      -2.1653639403     -0.7638042271      0.0000000000
H11      -2.1361992242      1.7106422948      0.0000000000
H12       0.0281645993      2.9675455950      0.0000000000
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  phen    1       1.2185  -0.2108   0.0000  -0.4062  1.500
ATOM      2  C2  phen    1       1.1753   1.1774   0.0000  -0.0531  1.500
ATOM      3  C3  phen    1      -0.0432   1.8790   0.0000  -0.3503  1.500
ATOM      4  C4  phen    1      -1.2282   1.1226   0.0000  -0.0530  1.500
ATOM      5  C5  phen    1      -1.2080  -0.2664   0.0000  -0.4067  1.500
ATOM      6  C6  phen    1       0.0235  -1.0353   0.0000   0.5941  1.500
ATOM      7  H7  phen    1       2.1749  -0.7350   0.0000   0.0970  1.200
ATOM      8  H8  phen    1       2.1138   1.7392   0.0000   0.0673  1.200
ATOM      9  H9  phen    1      -2.1920   1.6400   0.0000   0.0673  1.200
ATOM     10  H10 phen    1      -2.1393  -0.8339   0.0000   0.0970  1.200
ATOM     11  H11 phen    1      -0.0677   2.9678   0.0000   0.0924  1.200
ATOM     12  O12 phen    1       0.0535  -2.3016   0.0000  -0.7458  1.400
```

6 C.2.a) primary data for m-aminophenol

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1        1.2210635325      0.0328299486      2.1462850028
C2        0.0316882910     -0.0166665218      1.4105631001
C3        0.0537494758     -0.0440508639      0.0158503811
C4        1.2761308890     -0.0243356631     -0.6698982209
C5        2.4766592659      0.0298899745      0.0647621675
C6        2.4341398960      0.0575529079      1.4547363969
O7       -1.2000874295     -0.0419210420      2.0082184227
H8       -1.0780775183     -0.0090801651      2.9654904535
H9        1.2009843611      0.0490295142      3.2330321130
H10       3.3639712409      0.0911442453      2.0158041645
H11      -0.8892834285     -0.0713138301     -0.5223697413
H12       3.4288615764      0.0520624645     -0.4579272781
N13       1.2991085163      0.0019230246     -2.0649133564
H14       2.1539898834     -0.3346574844     -2.4860881071
H15       0.4796227144     -0.3809714757     -2.5160857216
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  phen    1      -0.8770  -0.4654   0.0000  -0.4816  1.500
ATOM      2  C2  phen    1      -0.8523   0.9388   0.0000   0.5603  1.500
ATOM      3  C3  phen    1       0.3908   1.6046   0.0000  -0.4201  1.500
ATOM      4  C4  phen    1       1.5689   0.8661   0.0000   0.0029  1.500
ATOM      5  C5  phen    1       1.5539  -0.5302   0.0000  -0.4478  1.500
ATOM      6  C6  phen    1       0.3162  -1.1858   0.0000   0.4514  1.500
ATOM      7  H7  phen    1       0.4214   2.6915   0.0000   0.1645  1.200
ATOM      8  H8  phen    1       2.5234   1.3867   0.0000   0.1252  1.200
ATOM      9  H9  phen    1       2.4816  -1.0987   0.0000   0.1639  1.200
ATOM     10  H10 phen    1      -1.8177  -1.0095   0.0000   0.2048  1.200
ATOM     11  N11 phen    1      -2.0302   1.6552   0.0000  -0.9949  1.400
ATOM     12  H12 phen    1      -2.0240   2.6610   0.0000   0.4194  1.200
ATOM     13  H13 phen    1      -2.9214   1.1886   0.0000   0.4127  1.200
ATOM     14  O14 phen    1       0.2156  -2.5529   0.0000  -0.5708  1.400
ATOM     15  H15 phen    1       1.1113  -2.9245   0.0000   0.4098  1.000
```

6 C.2.a) primary data for m-aminophenoxide

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1         2.4175786921      0.0507511702      1.4696642064
C2         1.2038931845      0.0070779092      2.1387871155
C3        -0.0654501471     -0.0350786193      1.4340090344
C4         0.0674336627     -0.0367340552     -0.0098319140
C5         1.2955045655      0.0057604212     -0.6602366011
C6         2.5014859101      0.0535010194      0.0666973494
O7        -1.1856456017     -0.0782086000      2.0227752583
H8         1.1702034990      0.0002927899      3.2274252746
H9         3.3422126859      0.0767535815      2.0510778024
H10       -0.8557478378     -0.0703933849     -0.5909957057
H11        3.4587115328      0.0967817970     -0.4496273735
N12        1.3461617376      0.0459659676     -2.0953417695
H13        2.1448754939     -0.4840615828     -2.4341177751
H14        0.5083228679     -0.3789577690     -2.4825748299
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ip172=2
basis=6-31g**
&

ATOM      1  C1  phen   1      -0.4892  -0.8704   0.0000  -0.6602  1.500
ATOM      2  C2  phen   1       0.9042  -0.8483   0.0000   0.6114  1.500
ATOM      3  C3  phen   1       1.6069   0.3758   0.0000  -0.5692  1.500
ATOM      4  C4  phen   1       0.8536   1.5630   0.0000  -0.0096  1.500
ATOM      5  C5  phen   1      -0.5319   1.5627   0.0000  -0.4980  1.500
ATOM      6  C6  phen   1      -1.3010   0.3284   0.0000   0.6563  1.500
ATOM      7  H7  phen   1       2.6968   0.3914   0.0000   0.1400  1.200
ATOM      8  H8  phen   1       1.3868   2.5180   0.0000   0.0770  1.200
ATOM      9  H9  phen   1      -1.0942   2.4962   0.0000   0.1129  1.200
ATOM     10  H10 phen   1      -1.0186  -1.8257   0.0000   0.1485  1.200
ATOM     11  N11 phen   1       1.6259  -2.0541   0.0000  -1.0424  1.400
ATOM     12  H12 phen   1       2.6309  -2.0535   0.0000   0.3857  1.200
ATOM     13  H13 phen   1       1.1439  -2.9360   0.0000   0.3923  1.200
ATOM     14  O14 phen   1      -2.5676   0.3032   0.0000  -0.7449  1.400
```

6 C.3.a) primary data for o-aminophenol

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1         0.8847024164     -0.1001130017      0.0000000000
C2         0.8765281219      1.3015714876      0.0000000000
C3        -0.3252392424      2.0140793858      0.0000000000
C4        -1.5458504975      1.3411333442      0.0000000000
C5        -1.5539560801     -0.0594395466      0.0000000000
C6        -0.3601648893     -0.7689607820      0.0000000000
H7         1.8265141376      1.8320261720      0.0000000000
H8        -0.3031611222      3.1005204098      0.0000000000
H9        -2.4844511076      1.8870729886      0.0000000000
H10       -2.4960321705     -0.6068587063      0.0000000000
N11        2.0423514143     -0.8466386367      0.0000000000
H12        2.9448907799     -0.4040145490      0.0000000000
H13        1.9877156452     -1.8506675451      0.0000000000
O14       -0.2876620428     -2.1473996853      0.0000000000
H15       -1.1880315573     -2.5056763997      0.0000000000
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  phen    1       0.8847  -0.1001   0.0000   0.3913  1.500
ATOM      2  C2  phen    1       0.8765   1.3016   0.0000  -0.3303  1.500
ATOM      3  C3  phen    1      -0.3252   2.0141   0.0000  -0.1492  1.500
ATOM      4  C4  phen    1      -1.5459   1.3411   0.0000  -0.1495  1.500
ATOM      5  C5  phen    1      -1.5540  -0.0594   0.0000  -0.3175  1.500
ATOM      6  C6  phen    1      -0.3602  -0.7690   0.0000   0.2338  1.500
ATOM      7  H7  phen    1       1.8265   1.8320   0.0000   0.1702  1.200
ATOM      8  H8  phen    1      -0.3032   3.1005   0.0000   0.1336  1.200
ATOM      9  H9  phen    1      -2.4845   1.8871   0.0000   0.1309  1.200
ATOM     10  H10 phen    1      -2.4960  -0.6069   0.0000   0.1623  1.200
ATOM     11  N11 phen    1       2.0424  -0.8466   0.0000  -0.9403  1.400
ATOM     12  H12 phen    1       2.9449  -0.4040   0.0000   0.3985  1.200
ATOM     13  H13 phen    1       1.9877  -1.8507   0.0000   0.4208  1.200
ATOM     14  O14 phen    1      -0.2877  -2.1474   0.0000  -0.5712  1.400
ATOM     15  H15 phen    1      -1.1880  -2.5057   0.0000   0.4166  1.000
```

6 C.3.b) primary data for o-aminophenoxide

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1       -0.0796302161      0.8778871693      0.0000000000
C2        1.3076495285      0.8620373585      0.0000000000
C3        2.0189890209     -0.3622806752      0.0000000000
C4        1.3001949412     -1.5551493622      0.0000000000
C5       -0.1058941945     -1.5545931555      0.0000000000
C6       -0.8720021261     -0.3550366421      0.0000000000
H7        1.8556620324      1.8091255842      0.0000000000
H8        3.1088298623     -0.3622888189      0.0000000000
H9        1.8321737092     -2.5095043951      0.0000000000
H10      -0.6606320230     -2.4935395802      0.0000000000
N11      -0.8724545395      2.0168886511      0.0000000000
H12      -0.5058266485      2.9513549441      0.0000000000
H13      -1.8634544160      1.8020821728      0.0000000000
O14      -2.1513628707     -0.2753134811      0.0000000000
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  phen   1      -0.0796   0.8779   0.0000   0.2119  1.500
ATOM      2  C2  phen   1       1.3076   0.8620   0.0000  -0.2839  1.500
ATOM      3  C3  phen   1       2.0190  -0.3623   0.0000  -0.3024  1.500
ATOM      4  C4  phen   1       1.3002  -1.5551   0.0000  -0.1319  1.500
ATOM      5  C5  phen   1      -0.1059  -1.5546   0.0000  -0.4382  1.500
ATOM      6  C6  phen   1      -0.8720  -0.3550   0.0000   0.4607  1.500
ATOM      7  H7  phen   1       1.8557   1.8091   0.0000   0.1128  1.200
ATOM      8  H8  phen   1       3.1088  -0.3623   0.0000   0.1002  1.200
ATOM      9  H9  phen   1       1.8322  -2.5095   0.0000   0.0811  1.200
ATOM     10  H10 phen   1      -0.6606  -2.4935   0.0000   0.1205  1.200
ATOM     11  N11 phen   1      -0.8725   2.0169   0.0000  -0.9272  1.400
ATOM     12  H12 phen   1      -0.5058   2.9514   0.0000   0.3620  1.200
ATOM     13  H13 phen   1      -1.8635   1.8021   0.0000   0.3670  1.200
ATOM     14  O14 phen   1      -2.1514  -0.2753   0.0000  -0.7325  1.400
```

6 C.4.a) primary data for m-chlorophenol

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
mulken=1
basis=cc-pvqz
&
&zmat
C1       -0.5062720807      0.7570072800      0.0000000000
C2       -0.4534843629     -0.6365669633      0.0000000000
C3        0.7567593176     -1.3258142591      0.0000000000
C4        1.9412032079     -0.5826231819      0.0000000000
C5        1.9221503521      0.8090785928      0.0000000000
C6        0.6928966942      1.4785500230      0.0000000000
H7       -1.4647001684      1.2677813482      0.0000000000
Cl       -1.9643055723     -1.5388129245      0.0000000000
H9        2.8943478343     -1.1029427430      0.0000000000
H10       2.8373675382      1.3908596497      0.0000000000
H11       0.7712735492     -2.4091888188      0.0000000000
O12       0.7224786490      2.8426286230      0.0000000000
H13      -0.1818005464      3.1826076263      0.0000000000
&
&atomic
atom    basis
Cl      6-31g**
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
```

```
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

6 C.4.a) primary data for m-chlorophenoxide

```
ATOM      1  C1  phen   1      -0.5063   0.7570   0.0000  -0.2985  1.500
ATOM      2  C2  phen   1      -0.4535  -0.6366   0.0000   0.1126  1.500
ATOM      3  C3  phen   1       0.7568  -1.3258   0.0000  -0.1395  1.500
ATOM      4  C4  phen   1       1.9412  -0.5826   0.0000  -0.1279  1.500
ATOM      5  C5  phen   1       1.9222   0.8091   0.0000  -0.2554  1.500
ATOM      6  C6  phen   1       0.6929   1.4786   0.0000   0.3838  1.500
ATOM      7  H7  phen   1      -1.4647   1.2678   0.0000   0.1481  1.200
ATOM      8  Cl  phen   1      -1.9643  -1.5388   0.0000  -0.1188  1.900
ATOM      9  H9  phen   1       2.8943  -1.1029   0.0000   0.1449  1.200
ATOM     10  H10 phen   1       2.8374   1.3909   0.0000   0.1716  1.200
ATOM     11  H11 phen   1       0.7713  -2.4092   0.0000   0.1235  1.200
ATOM     12  O12 phen   1       0.7225   2.8426   0.0000  -0.5654  1.400
ATOM     13  H13 phen   1      -0.1818   3.1826   0.0000   0.4210  1.000
```

6 C.4.b) primary data for m-chlorophenoxide

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
mulken=1
basis=cc-pvqz
&
&zmat
C1        0.7830170946     -0.5039059652      0.0000000000
C2       -0.5946108902     -0.4270171009      0.0000000000
C3       -1.3206302958      0.7680839067      0.0000000000
C4       -0.5536639743      1.9480713114      0.0000000000
C5        0.8319803308      1.9339737601      0.0000000000
C6        1.6013979835      0.7027986013      0.0000000000
H7        1.2942903079     -1.4610014353      0.0000000000
Cl       -1.5429117845     -1.9693170088      0.0000000000
```

```
H9       -1.0770934318                 2.9057181044      0.0000000000
H10       1.3969383939      2.8642891673      0.0000000000
H11      -2.4039940255      0.7763361220      0.0000000000
O12       2.8621604090      0.6674350931      0.0000000000
&
&atomic
atom    basis
Cl      6-31g**
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  phen    1       0.7830  -0.5039   0.0000  -0.4287  1.500
ATOM      2  C2  phen    1      -0.5946  -0.4270   0.0000   0.2106  1.500
ATOM      3  C3  phen    1      -1.3206   0.7681   0.0000  -0.3595  1.500
ATOM      4  C4  phen    1      -0.5537   1.9481   0.0000  -0.0610  1.500
ATOM      5  C5  phen    1       0.8320   1.9340   0.0000  -0.4322  1.500
ATOM      6  C6  phen    1       1.6014   0.7028   0.0000   0.5969  1.500
ATOM      7  H7  phen    1       1.2943  -1.4610   0.0000   0.1324  1.200
ATOM      8  Cl  phen    1      -1.5429  -1.9693   0.0000  -0.2636  1.900
ATOM      9  H9  phen    1      -1.0771   2.9057   0.0000   0.0894  1.200
ATOM     10  H10 phen    1       1.3969   2.8643   0.0000   0.1163  1.200
ATOM     11  H11 phen    1      -2.4040   0.7763   0.0000   0.1179  1.200
ATOM     12  O12 phen    1       2.8622   0.6674   0.0000  -0.7185  1.400
```

6 C.5.a) primary data for o-chlorophenol

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
mulken=1
basis=cc-pvqz
&
&zmat
C1       -0.4727858269      0.0969451271      0.0000000000
C2       -0.4521329595      1.4897350114      0.0000000000
C3        0.7712572677      2.1588867694      0.0000000000
C4        1.9611701261      1.4246810843      0.0000000000
C5        1.9351138043      0.0331396024      0.0000000000
C6        0.7140459202     -0.6524086703      0.0000000000
Cl       -2.0121299423     -0.7677707812      0.0000000000
H8       -1.3893264220      2.0357502376      0.0000000000
H9        2.9173203149      1.9390791130      0.0000000000
H10       2.8480959864     -0.5530934231      0.0000000000
H11       0.7917958353      3.2437207338      0.0000000000
O12       0.7406131097     -2.0084506089      0.0000000000
H13      -0.1711730127     -2.3380068114      0.0000000000
&
&atomic
atom    basis
Cl      6-31g**
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
```

```
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  phen    1      -0.4728   0.0969   0.0000  -0.0999  1.500
ATOM      2  C2  phen    1      -0.4521   1.4897   0.0000  -0.0570  1.500
ATOM      3  C3  phen    1       0.7713   2.1589   0.0000  -0.2027  1.500
ATOM      4  C4  phen    1       1.9612   1.4247   0.0000  -0.0897  1.500
ATOM      5  C5  phen    1       1.9351   0.0331   0.0000  -0.2750  1.500
ATOM      6  C6  phen    1       0.7140  -0.6524   0.0000   0.3940  1.500
ATOM      7  Cl  phen    1      -2.0121  -0.7678   0.0000  -0.0990  1.900
ATOM      8  H8  phen    1      -1.3893   2.0358   0.0000   0.1325  1.200
ATOM      9  H9  phen    1       2.9173   1.9391   0.0000   0.1298  1.200
ATOM     10  H10 phen    1       2.8481  -0.5531   0.0000   0.1754  1.200
ATOM     11  H11 phen    1       0.7918   3.2437   0.0000   0.1411  1.200
ATOM     12  O12 phen    1       0.7406  -2.0085   0.0000  -0.5341  1.400
ATOM     13  H13 phen    1      -0.1712  -2.3380   0.0000   0.3846  1.000
```

6 C.5.b) primary data for o-chlorophenoxide

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
mulken=1
basis=cc-pvqz
&
&zmat
C1       -0.4529371438      0.0723199865      0.0000000000
C2       -0.4295861813      1.4594764507      0.0000000000
C3        0.7890915527      2.1539734428      0.0000000000
C4        1.9741418517      1.3998446186      0.0000000000
C5        1.9492258905      0.0136749030      0.0000000000
C6        0.7298098068     -0.7759087154      0.0000000000
Cl       -2.0442063978     -0.7439260321      0.0000000000
H8       -1.3720760073      2.0036727444      0.0000000000
H9        2.9369974977      1.9140109024      0.0000000000
H10       2.8747721715     -0.5595542093      0.0000000000
H11       0.8067906603      3.2408268650      0.0000000000
O12       0.7176696562     -2.0329537547      0.0000000000
&
&atomic
atom    basis
Cl      6-31g**
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  phen   1      -0.4529   0.0723   0.0000  -0.0955  1.500
ATOM      2  C2  phen   1      -0.4296   1.4595   0.0000  -0.0954  1.500
ATOM      3  C3  phen   1       0.7891   2.1540   0.0000  -0.3459  1.500
ATOM      4  C4  phen   1       1.9741   1.3998   0.0000  -0.0533  1.500
ATOM      5  C5  phen   1       1.9492   0.0137   0.0000  -0.4490  1.500
ATOM      6  C6  phen   1       0.7298  -0.7759   0.0000   0.5809  1.500
ATOM      7  Cl  phen   1      -2.0442  -0.7439   0.0000  -0.2525  1.900
ATOM      8  H8  phen   1      -1.3721   2.0037   0.0000   0.0957  1.200
ATOM      9  H9  phen   1       2.9370   1.9140   0.0000   0.0811  1.200
ATOM     10  H10 phen   1       2.8748  -0.5596   0.0000   0.1245  1.200
ATOM     11  H11 phen   1       0.8068   3.2408   0.0000   0.1113  1.200
ATOM     12  O12 phen   1       0.7177  -2.0330   0.0000  -0.7019  1.400
```

6 D.1.a) primary data for glutarimide

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
  C1        0.0165372636     -0.2747795997      0.0193889005
  C2       -0.0006763205      0.2939220578      1.4423189286
  C3        1.2486658533      0.2266367041     -0.7401050381
  C4        2.5468546607     -0.0148906616      0.0110656384
  C5        1.2916224898      0.0302600989      2.1949850492
  N6        2.4305675972     -0.1212455111      1.3992922189
  O7        3.6346463421     -0.1002462541     -0.5244837391
  O8        1.3729861714     -0.0348523312      3.4058431039
  H9        3.3014323674     -0.2614476091      1.9026921613
  H10       0.0324225930     -1.3705189775      0.0615171674
  H11       1.1768226823      1.3098148585     -0.9114620988
  H12      -0.1374714354      1.3840084755      1.4138885262
  H13       1.3570324531     -0.2401420469     -1.7220549664
  H14      -0.8966319189      0.0087270856     -0.5122768766
  H15      -0.8131558078     -0.1111532342      2.0498205217
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  imid   1       0.0165  -0.2748   0.0194   0.0909  1.500
ATOM      2  C2  imid   1      -0.0007   0.2939   1.4423  -0.2493  1.500
ATOM      3  C3  imid   1       1.2487   0.2266  -0.7401  -0.2512  1.500
ATOM      4  C4  imid   1       2.5469  -0.0149   0.0111   0.6411  1.500
ATOM      5  C5  imid   1       1.2916   0.0303   2.1950   0.6397  1.500
ATOM      6  N6  imid   1       2.4306  -0.1212   1.3993  -0.6001  1.400
ATOM      7  O7  imid   1       3.6346  -0.1002  -0.5245  -0.5218  1.400
ATOM      8  O8  imid   1       1.3730  -0.0349   3.4058  -0.5204  1.400
ATOM      9  H9  imid   1       3.3014  -0.2614   1.9027   0.3558  1.000
ATOM     10  H10 imid   1       0.0324  -1.3705   0.0615   0.0230  1.200
ATOM     11  H11 imid   1       1.1768   1.3098  -0.9115   0.0978  1.200
ATOM     12  H12 imid   1      -0.1375   1.3840   1.4139   0.0974  1.200
ATOM     13  H13 imid   1       1.3570  -0.2401  -1.7221   0.0872  1.200
ATOM     14  H14 imid   1      -0.8966   0.0087  -0.5123   0.0235  1.200
ATOM     15  H15 imid   1      -0.8132  -0.1112   2.0498   0.0862  1.200
```

6 D.1.b) primary data for glutarimide deprotonated (anion)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
  C1       -0.0168239588     -0.2044948435      0.0043653378
  C2        0.0297746402      0.3449377055      1.4281526429
  C3        1.2474993974      0.2525563115     -0.7174942184
  C4        2.5428848918     -0.0183399641      0.0955824986
  C5        1.3553969665     -0.0181499279      2.1471090080
  N6        2.5058485595     -0.1698527774      1.4430152336
  O7        3.5944780723     -0.0699856765     -0.5640334719
  O8        1.2977716642     -0.1335627027      3.3826625540
  H9       -0.0396634270     -1.3032604079      0.0409421567
  H10       1.1947673785      1.3371374807     -0.9019637077
  H11      -0.0538818586      1.4428985006      1.3988676211
  H12       1.3749884889     -0.2228399474     -1.6959382985
  H13      -0.9272685409      0.1114184684     -0.5274852997
  H14      -0.7912333967     -0.0197945622      2.0538336044
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  imid   1      -0.0168  -0.2045   0.0044  0.1795   1.500
ATOM      2  C2  imid   1       0.0298   0.3449   1.4282 -0.3121   1.500
ATOM      3  C3  imid   1       1.2475   0.2526  -0.7175 -0.3148   1.500
ATOM      4  C4  imid   1       2.5429  -0.0183   0.0956  0.8057   1.500
ATOM      5  C5  imid   1       1.3554  -0.0181   2.1471  0.8031   1.500
ATOM      6  N6  imid   1       2.5058  -0.1699   1.4430 -0.8874   1.400
ATOM      7  O7  imid   1       3.5945  -0.0700  -0.5640 -0.6890   1.400
ATOM      8  O8  imid   1       1.2978  -0.1336   3.3827 -0.6858   1.400
ATOM      9  H9  imid   1      -0.0397  -1.3033   0.0409 -0.0274   1.200
ATOM     10  H10 imid   1       1.1948   1.3371  -0.9020  0.0550   1.200
ATOM     11  H11 imid   1      -0.0539   1.4429   1.3989  0.0556   1.200
ATOM     12  H12 imid   1       1.3750  -0.2228  -1.6959  0.0360   1.200
ATOM     13  H13 imid   1      -0.9273   0.1114  -0.5275 -0.0509   1.200
ATOM     14  H14 imid   1      -0.7912  -0.0198   2.0538  0.0326   1.200
```

6 D.2.a) primary data for glutaconimide

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1        0.0804821888     -0.0301345307     -0.0362591875
C2       -0.0108329354     -0.0503845550      1.4593429857
C3        1.2463604641      0.0194618030     -0.6902329207
C4        2.5381094020      0.0636414331      0.0248199390
C5        1.3141349631     -0.0430870076      2.2093530899
N6        2.4556161704      0.0357171168      1.4247741081
O7        3.6208763639      0.1228777553     -0.5309098456
O8        1.3782978960     -0.0925456822      3.4225671144
H9        3.3406186032      0.0523652209      1.9216533168
H10      -0.8557012063     -0.0535223681     -0.5883298748
H11       1.3170574725      0.0416036826     -1.7712416970
H12      -0.5880937121      0.8116497142      1.8212405294
H13      -0.5726524411     -0.9275928108      1.8054827195
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  mfn2   1       0.0805  -0.0301  -0.0363   0.0217 1.500
ATOM      2  C2  mfn2   1      -0.0108  -0.0504   1.4593  -0.1965 1.500
ATOM      3  C3  mfn2   1       1.2464   0.0195  -0.6902  -0.4414 1.500
ATOM      4  C4  mfn2   1       2.5381   0.0636   0.0248   0.7688 1.500
ATOM      5  C5  mfn2   1       1.3141  -0.0431   2.2094   0.6855 1.500
ATOM      6  N6  mfn2   1       2.4556   0.0357   1.4248  -0.6393 1.400
ATOM      7  O7  mfn2   1       3.6209   0.1229  -0.5309  -0.5327 1.400
ATOM      8  O8  mfn2   1       1.3783  -0.0925   3.4226  -0.5405 1.400
ATOM      9  H9  mfn2   1       3.3406   0.0524   1.9217   0.3579 1.000
ATOM     10  H10 mfn2   1      -0.8557  -0.0535  -0.5883   0.1208 1.200
ATOM     11  H11 mfn2   1       1.3171   0.0416  -1.7712   0.1895 1.200
ATOM     12  H12 mfn2   1      -0.5881   0.8116   1.8212   0.1041 1.200
ATOM     13  H13 mfn2   1      -0.5727  -0.9276   1.8055   0.1020 1.200
```

6 D.2.b) primary data for glutaconimide deprotonated (anion)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
  C1       -0.0293628406      0.0518529363      0.0635865804
  C2        0.0339988685     -0.0077332009      1.3953704598
  C3        1.2398086924      0.0715131881     -0.7318075675
  C4        2.5541771699      0.0294228333      0.1049896590
  C5        1.3516359770     -0.0558827185      2.1337731746
  N6        2.5300026954     -0.0290499131      1.4561401951
  O7        3.6002870243      0.0531937611     -0.5650419715
  O8        1.2786463466     -0.1114992693      3.3761331518
  H9        1.2900143175      0.9626098604     -1.3743289776
  H10       1.2784223242     -0.7769224823     -1.4319572365
  H11      -0.9842290100      0.0992742434     -0.4653228640
  H12      -0.8498653293     -0.0177493186      2.0295335922
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=-1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  mfn2   1      -0.0294   0.0519   0.0636   0.0144 1.500
ATOM      2  C2  mfn2   1       0.0340  -0.0077   1.3954  -0.4996 1.500
ATOM      3  C3  mfn2   1       1.2398   0.0715  -0.7318  -0.2850 1.500
ATOM      4  C4  mfn2   1       2.5542   0.0294   0.1050   0.8476 1.500
ATOM      5  C5  mfn2   1       1.3516  -0.0559   2.1338   0.9217 1.500
ATOM      6  N6  mfn2   1       2.5300  -0.0290   1.4561  -0.9206 1.400
ATOM      7  O7  mfn2   1       3.6003   0.0532  -0.5650  -0.7071 1.400
ATOM      8  O8  mfn2   1       1.2786  -0.1115   3.3761  -0.6951 1.400
ATOM      9  H9  mfn2   1       1.2900   0.9626  -1.3743   0.0625 1.200
ATOM     10  H10 mfn2   1       1.2784  -0.7769  -1.4320   0.0618 1.200
ATOM     11  H11 mfn2   1      -0.9842   0.0993  -0.4653   0.0598 1.200
ATOM     12  H12 mfn2   1      -0.8499  -0.0177   2.0295   0.1398 1.200
```

6 E.1.a) primary data for pyridine protonated (cation)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
  C1       -0.6561634969      1.1965000641      0.0000000000
  C2        0.7277395776      1.2072496875      0.0000000000
  C3        1.4176260900     -0.0114007485      0.0000000000
  C4        0.7084231206     -1.2175760117      0.0000000000
  C5       -0.6763271479     -1.1857988447      0.0000000000
  N6       -1.3092104616      0.0096089788      0.0000000000
  H7       -1.2691339729      2.0900510451      0.0000000000
  H8        1.2531076146      2.1553895984      0.0000000000
  H9        2.5030969888     -0.0205507631      0.0000000000
  H10       1.2179176148     -2.1744125781      0.0000000000
  H11      -1.3003574162     -2.0717201415      0.0000000000
  H12      -2.3278384708      0.0190152680      0.0000000000
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  pyri   1      -0.6562   1.1965   0.0000  0.0390  1.500
ATOM      2  C2  pyri   1       0.7277   1.2072   0.0000 -0.1194  1.500
ATOM      3  C3  pyri   1       1.4176  -0.0114   0.0000  0.0562  1.500
ATOM      4  C4  pyri   1       0.7084  -1.2176   0.0000 -0.1197  1.500
ATOM      5  C5  pyri   1      -0.6763  -1.1858   0.0000  0.0399  1.500
ATOM      6  N6  pyri   1      -1.3092   0.0096   0.0000 -0.1275  1.400
ATOM      7  H7  pyri   1      -1.2691   2.0901   0.0000  0.1830  1.200
ATOM      8  H8  pyri   1       1.2531   2.1554   0.0000  0.1801  1.200
ATOM      9  H9  pyri   1       2.5031  -0.0206   0.0000  0.1611  1.200
ATOM     10  H10 pyri   1       1.2179  -2.1744   0.0000  0.1801  1.200
ATOM     11  H11 pyri   1      -1.3004  -2.0717   0.0000  0.1829  1.200
ATOM     12  H12 pyri   1      -2.3278   0.0190   0.0000  0.3441  1.000
```

6 E.1.b) primary data for pyridine (neutral)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
  C1       -0.6941518964      1.1436085213      0.0000000000
  C2        0.7007348866      1.1997381501      0.0000000000
  C3        1.4133864143      0.0001953847      0.0000000000
  C4        0.7015056317     -1.1992900114      0.0000000000
  C5       -0.6939988451     -1.1435334751      0.0000000000
  N6       -1.3930651419     -0.0007090833      0.0000000000
  H7       -1.2830553631      2.0597607263      0.0000000000
  H8        1.2111824209      2.1585657477      0.0000000000
  H9        2.5000460578      0.0014306266      0.0000000000
  H10       1.2124364355     -2.1578199082      0.0000000000
  H11      -1.2815889792     -2.0606408253      0.0000000000
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  pyri   1      -0.6942   1.1436   0.0000  0.4651   1.500
ATOM      2  C2  pyri   1       0.7007   1.1997   0.0000 -0.4670   1.500
ATOM      3  C3  pyri   1       1.4134   0.0002   0.0000  0.2027   1.500
ATOM      4  C4  pyri   1       0.7015  -1.1993   0.0000 -0.4672   1.500
ATOM      5  C5  pyri   1      -0.6940  -1.1435   0.0000  0.4655   1.500
ATOM      6  N6  pyri   1      -1.3931  -0.0007   0.0000 -0.6461   1.400
ATOM      7  H7  pyri   1      -1.2831   2.0598   0.0000  0.0133   1.200
ATOM      8  H8  pyri   1       1.2112   2.1586   0.0000  0.1692   1.200
ATOM      9  H9  pyri   1       2.5000   0.0014   0.0000  0.0819   1.200
ATOM     10  H10 pyri   1       1.2124  -2.1578   0.0000  0.1693   1.200
ATOM     11  H11 pyri   1      -1.2816  -2.0606   0.0000  0.0131   1.200
```

6 E.2.a) primary data for 2-methylpyridine (cation)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C      1.2454330187     -0.1754394442      0.0000000000
C      1.1766820251      1.2161544584      0.0000000000
C     -0.0689880502      1.8621759849      0.0000000000
C     -1.2116088448      1.0896274720      0.0000000000
N     -1.1001385273     -0.2637892249      0.0000000000
C      0.0776121933     -0.9375513707      0.0000000000
H      2.0902327856      1.8019977834      0.0000000000
H     -0.1502990873      2.9424241267      0.0000000000
H     -2.2173471190      1.4914486243      0.0000000000
H     -1.9573304420     -0.8113272614      0.0000000000
H      2.2028100952     -0.6843893873      0.0000000000
C      0.0522692273     -2.4337810043      0.0000000000
H     -0.9656594003     -2.8308324092      0.0000000000
H      0.5724831739     -2.8202490083     -0.8821264350
H      0.5724831739     -2.8202490083      0.8821264350
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  pyri   1      -0.4579   0.8242   0.0000  0.3837  1.500
ATOM      2  C2  pyri   1       0.9335   0.8498   0.0000 -0.2282  1.500
ATOM      3  C3  pyri   1       1.6612  -0.3431   0.0000  0.0511  1.500
ATOM      4  C4  pyri   1       0.9976  -1.5758   0.0000 -0.1601  1.500
ATOM      5  C5  pyri   1      -0.3851  -1.5797   0.0000  0.0411  1.500
ATOM      6  N6  pyri   1      -1.0529  -0.4026   0.0000 -0.2008  1.400
ATOM      7  H7  pyri   1       1.4393   1.8089   0.0000  0.1851  1.200
ATOM      8  H8  pyri   1       2.7463  -0.3103   0.0000  0.1642  1.200
ATOM      9  H9  pyri   1       1.5381  -2.5149   0.0000  0.1842  1.200
ATOM     10  H10 pyri   1      -0.9867  -2.4811   0.0000  0.1848  1.200
ATOM     11  H11 pyri   1      -2.0713  -0.4334   0.0000  0.3478  1.000
ATOM     12  C12 pyri   1      -1.3469   2.0328   0.0000 -0.5428  2.000
ATOM     13  H13 pyri   1      -0.7516   2.9478   0.0000  0.2054  1.200
ATOM     14  H14 pyri   1      -1.9908   2.0485  -0.8880  0.1920  1.200
ATOM     15  H15 pyri   1      -1.9908   2.0485   0.8880  0.1920  1.200
```

6 E.2.b) primary data for 2-methylpyridine deprotonated (neutral)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C     1.2286883181     -0.1662317737      0.0000000000
C     1.1685713168      1.2237287437      0.0000000000
C    -0.0834980685      1.8417041431      0.0000000000
C    -1.2129760113      1.0259344928      0.0000000000
N    -1.1677373740     -0.3130170772      0.0000000000
C     0.0368625620     -0.9052045606      0.0000000000
H     2.0800532336      1.8146308980      0.0000000000
H    -0.1852324923      2.9219829405      0.0000000000
H    -2.2089204970      1.4659801909      0.0000000000
H     2.1871685850     -0.6781501653      0.0000000000
C     0.0530536069     -2.4132488088      0.0000000000
H    -0.9716609118     -2.7875926167      0.0000000000
H     0.5730313701     -2.8056718962     -0.8815581298
H     0.5730313701     -2.8056718962      0.8815581298
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
```

```
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  pyri   1      -0.4838   0.7677   0.0000   0.7603  1.500
ATOM      2  C2  pyri   1       0.9127   0.8449   0.0000  -0.5250  1.500
ATOM      3  C3  pyri   1       1.6623  -0.3327   0.0000   0.1732  1.500
ATOM      4  C4  pyri   1       0.9952  -1.5550   0.0000  -0.4548  1.500
ATOM      5  C5  pyri   1      -0.4025  -1.5341   0.0000   0.3943  1.500
ATOM      6  N6  pyri   1      -1.1313  -0.4153   0.0000  -0.6670  1.400
ATOM      7  H7  pyri   1       1.4041   1.8143   0.0000   0.1743  1.200
ATOM      8  H8  pyri   1       2.7483  -0.2903   0.0000   0.0914  1.200
ATOM      9  H9  pyri   1       1.5342  -2.4976   0.0000   0.1662  1.200
ATOM     10  H10 pyri   1      -0.9650  -2.4679   0.0000   0.0332  1.200
ATOM     11  C11 pyri   1      -1.3579   2.0007   0.0000  -0.6601  2.000
ATOM     12  H12 pyri   1      -0.7694   2.9239   0.0000   0.1555  1.200
ATOM     13  H13 pyri   1      -2.0105   2.0035  -0.8805   0.1792  1.200
ATOM     14  H14 pyri   1      -2.0105   2.0035   0.8805   0.1792  1.200
```

6 E.3.a) primary data for 4-methylpyridine (cation)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1        0.0799981077     -0.0038212286      1.4393873836
C2        0.0519687413      0.0047177089      0.0582236926
C3        1.2520475893      0.0081611496     -0.6805215261
C4        2.4638646055      0.0063092192      0.0405413593
C5        2.4553213835     -0.0024847691      1.4212588654
N6        1.2722672276     -0.0071751807      2.0819995270
H7       -0.8113746252     -0.0060651526      2.0552361063
H8       -0.9077307141      0.0108434055     -0.4463246691
H9        3.4161563671      0.0134911023     -0.4777029517
H10       3.3540417908     -0.0034073988      2.0262110679
H11       1.2822494875     -0.0110899601      3.0983069035
C12       1.2387859117     -0.0045151677     -2.1800762706
```

```
H13       0.3460951186                  0.4857394389     -2.5778570774
H14       2.1288414559      0.4771425852     -2.5943786224
H15       1.2310322252     -1.0429509366     -2.5363108276
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  pyri   1       0.0800  -0.0038   1.4394  0.0456  1.500
ATOM      2  C2  pyri   1       0.0520   0.0047   0.0582 -0.2265  1.500
ATOM      3  C3  pyri   1       1.2520   0.0082  -0.6805  0.3951  1.500
ATOM      4  C4  pyri   1       2.4639   0.0063   0.0405 -0.2274  1.500
ATOM      5  C5  pyri   1       2.4553  -0.0025   1.4213  0.0456  1.500
ATOM      6  N6  pyri   1       1.2723  -0.0072   2.0820 -0.1617  1.400
ATOM      7  H7  pyri   1      -0.8114  -0.0061   2.0552  0.1867  1.200
ATOM      8  H8  pyri   1      -0.9077   0.0108  -0.4463  0.1903  1.200
ATOM      9  H9  pyri   1       3.4162   0.0135  -0.4777  0.1908  1.200
ATOM     10  H10 pyri   1       3.3540  -0.0034   2.0262  0.1865  1.200
ATOM     11  H11 pyri   1       1.2822  -0.0111   3.0983  0.3491  1.000
ATOM     12  C12 pyri   1       1.2388  -0.0045  -2.1801 -0.5446  2.000
ATOM     13  H13 pyri   1       0.3461   0.4857  -2.5779  0.1877  1.200
ATOM     14  H14 pyri   1       2.1288   0.4771  -2.5944  0.1875  1.200
ATOM     15  H15 pyri   1       1.2310  -1.0430  -2.5363  0.1950  1.200
```

6 E.3.b) primary data for 4- methylpyridine deprotonated (anion)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C1        0.1178343199     -0.0032893826      1.4321223042
C2        0.0647360381      0.0057126800      0.0384420618
C3        1.2572180911      0.0080478608     -0.6949025448
C4        2.4495560916      0.0070646629      0.0378816809
C5        2.3966485998     -0.0021545802      1.4319276955
N6        1.2575807154     -0.0074623030      2.1366995625
H7       -0.8033785471     -0.0040836956      2.0126029764
H8       -0.8960802258      0.0130808434     -0.4692212729
H9        3.4104619378      0.0152658913     -0.4696099486
H10       3.3183523452     -0.0018891536      2.0116898360
C11       1.2559131216     -0.0092948320     -2.2025956828
H12       0.3702951084      0.4897035580     -2.6062734537
H13       2.1446914513      0.4824843070     -2.6082170928
H14       1.2513940412     -1.0397157268     -2.5787975102
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  pyri   1       0.1178  -0.0033   1.4321  0.4705  1.500
ATOM      2  C2  pyri   1       0.0647   0.0057   0.0384 -0.6036  1.500
ATOM      3  C3  pyri   1       1.2572   0.0080  -0.6949  0.5926  1.500
ATOM      4  C4  pyri   1       2.4496   0.0071   0.0379 -0.6040  1.500
ATOM      5  C5  pyri   1       2.3966  -0.0022   1.4319  0.4708  1.500
ATOM      6  N6  pyri   1       1.2576  -0.0075   2.1367 -0.6616  1.400
ATOM      7  H7  pyri   1      -0.8034  -0.0041   2.0126  0.0209  1.200
ATOM      8  H8  pyri   1      -0.8961   0.0131  -0.4692  0.1921  1.200
ATOM      9  H9  pyri   1       3.4105   0.0153  -0.4696  0.1923  1.200
ATOM     10  H10 pyri   1       3.3184  -0.0019   2.0117  0.0209  1.200
ATOM     11  C11 pyri   1       1.2559  -0.0093  -2.2026 -0.5163  2.000
ATOM     12  H12 pyri   1       0.3703   0.4897  -2.6063  0.1396  1.200
ATOM     13  H13 pyri   1       2.1447   0.4825  -2.6082  0.1395  1.200
ATOM     14  H14 pyri   1       1.2514  -1.0397  -2.5788  0.1460  1.200
```

6 E.4.a) primary data for 2-aminopyridine (cation)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C     0.0255484875      0.0651937298      1.4366980815
C     0.0312267772      0.0173997835      0.0228604027
C     1.2292914734     -0.0642669108     -0.6528564699
C     2.4600347113     -0.1008293115      0.0461575059
C     2.4312055021     -0.0535682747      1.4114892508
N     1.2313294024      0.0287444644      2.0696709368
H    -0.9151968789      0.0479079447     -0.5043381929
H     1.2259440408     -0.0985824454     -1.7374303791
H     3.4064045191     -0.1643728171     -0.4753599369
H     3.3111852288     -0.0756692344      2.0419437216
H     1.2534052415      0.0540866410      3.0840734164
N    -1.0977911703      0.1461250194      2.1674649147
H    -1.9965801057      0.1769400022      1.7094775643
H    -1.0985968139      0.2005179407      3.1755308064
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  pyri   1       0.0255   0.0652   1.4367  0.6991 1.500
ATOM      2  C2  pyri   1       0.0312   0.0174   0.0229 -0.3695 1.500
ATOM      3  C3  pyri   1       1.2293  -0.0643  -0.6529  0.0925 1.500
ATOM      4  C4  pyri   1       2.4600  -0.1008   0.0462 -0.2101 1.500
ATOM      5  C5  pyri   1       2.4312  -0.0536   1.4115  0.0286 1.500
ATOM      6  N6  pyri   1       1.2313   0.0287   2.0697 -0.3246 1.400
ATOM      7  H7  pyri   1      -0.9152   0.0479  -0.5043  0.2084 1.200
ATOM      8  H8  pyri   1       1.2259  -0.0986  -1.7374  0.1632 1.200
ATOM      9  H9  pyri   1       3.4064  -0.1644  -0.4754  0.1894 1.200
ATOM     10  H10 pyri   1       3.3112  -0.0757   2.0419  0.1919 1.200
ATOM     11  H11 pyri   1       1.2534   0.0541   3.0841  0.3676 1.000
ATOM     12  N12 pyri   1      -1.0978   0.1461   2.1675 -1.0000 1.400
ATOM     13  H13 pyri   1      -1.9966   0.1769   1.7095  0.4880 1.200
ATOM     14  H14 pyri   1      -1.0986   0.2005   3.1755  0.4752 1.200
```

6 E.4.b) primary data for 2-aminopyridine deprotonated(neutral)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C    0.0661837918      0.0389008796      1.4114514747
C    0.0441703064     -0.0052432934      0.0010735097
C    1.2548750655     -0.0406479725     -0.6747976305
C    2.4521726951     -0.0420198059      0.0510442364
C    2.3621578508     -0.0033816370      1.4397409839
N    1.2077558050      0.0421020402      2.1175860563
H   -0.9010819941     -0.0164532189     -0.5332672466
H    1.2680120115     -0.0690770915     -1.7608371831
H    3.4175300914     -0.0684822774     -0.4419420033
H    3.2644366273     -0.0019170858      2.0495654900
N   -1.1061305344      0.0299090152      2.1490262540
H   -1.9215038135      0.4416630230      1.7187983454
H   -0.9728290320      0.2878923584      3.1176898117
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  pyri   1       0.0662   0.0389   1.4115  0.8244  1.500
ATOM      2  C2  pyri   1       0.0442  -0.0052   0.0011 -0.5562  1.500
ATOM      3  C3  pyri   1       1.2549  -0.0406  -0.6748  0.1659  1.500
ATOM      4  C4  pyri   1       2.4522  -0.0420   0.0510 -0.4696  1.500
ATOM      5  C5  pyri   1       2.3622  -0.0034   1.4397  0.3734  1.500
ATOM      6  N6  pyri   1       1.2078   0.0421   2.1176 -0.6678  1.400
ATOM      7  H7  pyri   1      -0.9011  -0.0165  -0.5333  0.1944  1.200
ATOM      8  H8  pyri   1       1.2680  -0.0691  -1.7608  0.0953  1.200
ATOM      9  H9  pyri   1       3.4175  -0.0685  -0.4419  0.1670  1.200
ATOM     10  H10 pyri   1       3.2644  -0.0019   2.0496  0.0416  1.200
ATOM     11  N11 pyri   1      -1.1061   0.0299   2.1490 -0.8971  1.400
ATOM     12  H12 pyri   1      -1.9215   0.4417   1.7188  0.3602  1.200
ATOM     13  H13 pyri   1      -0.9728   0.2879   3.1177  0.3683  1.200
```

6 E.5.a) primary data for 4- aminopyridine (cation)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C     0.0810369024     -0.0573472016      1.4081715386
C     0.0382318016      0.0256712724      0.0432619464
C     1.2511797232      0.0696549379     -0.7042563155
C     2.4761214703      0.0251704197      0.0237384428
C     2.4548233858     -0.0576188766      1.3891271670
N     1.2731529449     -0.0978858237      2.0620425714
H    -0.8109674699     -0.0938736665      2.0214046307
H    -0.9228033726      0.0568650089     -0.4570089981
H     3.4290040724      0.0557110567     -0.4918795287
H     3.3562911890     -0.0948842887      1.9883214547
H     1.2825485820     -0.1599687171      3.0737334966
N     1.2402677078      0.1508407703     -2.0401485908
H     0.3748398604      0.1909721093     -2.5590866207
H     2.0969890965      0.1939035869     -2.5730952545
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  pyri   1       0.0810  -0.0573   1.4082  0.0764  1.500
ATOM      2  C2  pyri   1       0.0382   0.0257   0.0433 -0.3630  1.500
ATOM      3  C3  pyri   1       1.2512   0.0697  -0.7043  0.6871  1.500
ATOM      4  C4  pyri   1       2.4761   0.0252   0.0237 -0.3630  1.500
ATOM      5  C5  pyri   1       2.4548  -0.0576   1.3891  0.0761  1.500
ATOM      6  N6  pyri   1       1.2732  -0.0979   2.0620 -0.2256  1.400
ATOM      7  H7  pyri   1      -0.8110  -0.0939   2.0214  0.1836  1.200
ATOM      8  H8  pyri   1      -0.9228   0.0569  -0.4570  0.2096  1.200
ATOM      9  H9  pyri   1       3.4290   0.0557  -0.4919  0.2097  1.200
ATOM     10  H10 pyri   1       3.3563  -0.0949   1.9883  0.1837  1.200
ATOM     11  H11 pyri   1       1.2825  -0.1600   3.0737  0.3508  1.000
ATOM     12  N12 pyri   1       1.2403   0.1508  -2.0401 -0.9612  1.400
ATOM     13  H13 pyri   1       0.3748   0.1910  -2.5591  0.4677  1.200
ATOM     14  H14 pyri   1       2.0970   0.1939  -2.5731  0.4677  1.200
```

6 E.5.b) primary data for 4-aminopyridine deprotonated (neutral)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C      0.1205739549     -0.0289628153      1.4105183751
C      0.0577639102      0.0175863760      0.0219199818
C      1.2564956100      0.0467996964     -0.7125878259
C      2.4559815829      0.0178071479      0.0210440954
C      2.3945311098     -0.0288720409      1.4095756025
N      1.2578031203     -0.0501940125      2.1218854222
H     -0.8040820366     -0.0463754820      1.9857767420
H     -0.9032678108      0.0299044801     -0.4849932630
H      3.4167316446      0.0304073346     -0.4864219513
H      3.3194312345     -0.0461993286      1.9843553845
N      1.2560825015      0.0457190642     -2.0965496872
H      0.4145738384      0.3786328204     -2.5455696906
H      2.0985369007      0.3761268060     -2.5456292642
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  pyri   1       0.1206  -0.0290   1.4105  0.4695  1.500
ATOM      2  C2  pyri   1       0.0578   0.0176   0.0219 -0.6459  1.500
ATOM      3  C3  pyri   1       1.2565   0.0468  -0.7126  0.7113  1.500
ATOM      4  C4  pyri   1       2.4560   0.0178   0.0210 -0.6450  1.500
ATOM      5  C5  pyri   1       2.3945  -0.0289   1.4096  0.4688  1.500
ATOM      6  N6  pyri   1       1.2578  -0.0502   2.1219 -0.6777  1.400
ATOM      7  H7  pyri   1      -0.8041  -0.0464   1.9858  0.0235  1.200
ATOM      8  H8  pyri   1      -0.9033   0.0299  -0.4850  0.2064  1.200
ATOM      9  H9  pyri   1       3.4167   0.0304  -0.4864  0.2059  1.200
ATOM     10  H10 pyri   1       3.3194  -0.0462   1.9844  0.0237  1.200
ATOM     11  N11 pyri   1       1.2561   0.0457  -2.0965 -0.8774  1.400
ATOM     12  H12 pyri   1       0.4146   0.3786  -2.5456  0.3683  1.200
ATOM     13  H13 pyri   1       2.0985   0.3761  -2.5456  0.3685  1.200
```

6 E.5.a) primary data for 3-chloropyridine (cation)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
  C1        1.1294984542     -0.3843984815      0.0000000000
  C2       -0.2612365878     -0.3955076976      0.0000000000
  C3       -0.9517379328      0.8271617763      0.0000000000
  C4       -0.2388029313      2.0267568168      0.0000000000
  C5        1.1469572489      1.9996429950      0.0000000000
  N6        1.7742317485      0.8022807593      0.0000000000
  H7        1.7339123355     -1.2829477525      0.0000000000
  Cl       -1.0945584449     -1.8979144624      0.0000000000
  H9       -2.0368070641      0.8309742998      0.0000000000
  H10      -0.7542348145      2.9801582761      0.0000000000
  H11       1.7722873824      2.8838124179      0.0000000000
  H12       2.7920139762      0.7891084403      0.0000000000
&
&atomic
atom    basis
Cl     6-31g**
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  pyri   1       1.1295  -0.3844   0.0000  0.1510  1.500
ATOM      2  C2  pyri   1      -0.2612  -0.3955   0.0000 -0.0971  1.500
ATOM      3  C3  pyri   1      -0.9517   0.8272   0.0000  0.1478  1.500
ATOM      4  C4  pyri   1      -0.2388   2.0268   0.0000 -0.1672  1.500
ATOM      5  C5  pyri   1       1.1470   1.9996   0.0000  0.0489  1.500
ATOM      6  N6  pyri   1       1.7742   0.8023   0.0000 -0.1584  1.400
ATOM      7  H7  pyri   1       1.7339  -1.2829   0.0000  0.1491  1.200
ATOM      8  Cl  pyri   1      -1.0946  -1.8979   0.0000  0.0558  1.900
ATOM      9  H9  pyri   1      -2.0368   0.8310   0.0000  0.1323  1.200
ATOM     10  H10 pyri   1      -0.7542   2.9802   0.0000  0.1941  1.200
ATOM     11  H11 pyri   1       1.7723   2.8838   0.0000  0.1848  1.200
ATOM     12  H12 pyri   1       2.7920   0.7891   0.0000  0.3586  1.000
```

6 E.5.b) primary data for 3- chloropyridine deprotonated(neutral)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
  C1        1.1620462461     -0.3191026837      0.0000000000
  C2       -0.2348846079     -0.3635382490      0.0000000000
  C3       -0.9606865073      0.8254536958      0.0000000000
  C4       -0.2463476044      2.0221764634      0.0000000000
  C5        1.1481912707      1.9725231151      0.0000000000
  N6        1.8447132986      0.8285508727      0.0000000000
  H7        1.7388526408     -1.2406901368      0.0000000000
  Cl       -1.0557889941     -1.9083115199      0.0000000000
  H9       -2.0450675805      0.8113271161      0.0000000000
  H10      -0.7638598098      2.9761914486      0.0000000000
  H11       1.7331337095      2.8896878292      0.0000000000
&
&atomic
atom    basis
Cl     6-31g**
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  C1  pyri   1       1.1620  -0.3191   0.0000  0.3250  1.500
ATOM      2  C2  pyri   1      -0.2349  -0.3635   0.0000 -0.0874  1.500
ATOM      3  C3  pyri   1      -0.9607   0.8255   0.0000  0.0058  1.500
ATOM      4  C4  pyri   1      -0.2463   2.0222   0.0000 -0.2187  1.500
ATOM      5  C5  pyri   1       1.1482   1.9725   0.0000  0.2344  1.500
ATOM      6  N6  pyri   1       1.8447   0.8286   0.0000 -0.5154  1.400
ATOM      7  H7  pyri   1       1.7389  -1.2407   0.0000  0.0420  1.200
ATOM      8  Cl  pyri   1      -1.0558  -1.9083   0.0000 -0.1026  1.900
ATOM      9  H9  pyri   1      -2.0451   0.8113   0.0000  0.1244  1.200
ATOM     10  H10 pyri   1      -0.7639   2.9762   0.0000  0.1256  1.200
ATOM     11  H11 pyri   1       1.7331   2.8897   0.0000  0.0667  1.200
```

6 F.1.a) primary data for imidazole protonated(cation)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C   1.132371    0.000000   -0.115452
N   0.237604    0.000000   -1.100248
C  -1.038894    0.000000   -0.575896
C  -0.901259    0.000000    0.773651
N   0.454842    0.000000    1.029702
H   0.879876    0.000000    1.946039
H  -1.635384    0.000000    1.558106
H  -1.916267    0.000000   -1.196007
H   2.202471    0.000000   -0.224615
H   0.468872    0.000000   -2.083518
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  N1  idaz   1       1.0639   0.3789   0.0000 -0.1187  1.400
ATOM      2  C2  idaz   1      -0.0320   1.1439   0.0000  0.0345  1.500
ATOM      3  N3  idaz   1      -1.0836   0.3182   0.0000 -0.1187  1.400
ATOM      4  C4  idaz   1      -0.6541  -0.9978   0.0000 -0.1037  1.500
ATOM      5  C5  idaz   1       0.7091  -0.9595   0.0000 -0.1038  1.500
ATOM      6  H6  idaz   1       2.0135   0.7377   0.0000  0.3601  1.000
ATOM      7  H7  idaz   1      -2.0516   0.6237   0.0000  0.3602  1.200
ATOM      8  H8  idaz   1      -1.3383  -1.8320   0.0000  0.2323  1.200
ATOM      9  H9  idaz   1       1.4393  -1.7537   0.0000  0.2324  1.200
ATOM     10  H10 idaz   1      -0.0628   2.2235   0.0000  0.2254  1.200
```

6 F.1.b) primary data for imidazole(neutral)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
C  -0.992687    0.000000   -0.619410
C  -0.884484    0.000000    0.743122
N   0.253450    0.000000   -1.201493
N   0.468097    0.000000    0.997434
C   1.106145    0.000000   -0.207012
H   0.902686    0.000000    1.903250
H  -1.616588    0.000000    1.529879
H  -1.890667    0.000000   -1.212798
H   2.179904    0.000000   -0.292119
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
```

```
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  N1  idaz   1       1.0811   0.3276   0.0000 -0.2077  1.400
ATOM      2  C2  idaz   1      -0.0375   1.1157   0.0000  0.2369  1.500
ATOM      3  N3  idaz   1      -1.1391   0.3971   0.0000 -0.5611  1.400
ATOM      4  C4  idaz   1      -0.7158  -0.9157   0.0000  0.2104  1.500
ATOM      5  C5  idaz   1       0.6550  -0.9863   0.0000 -0.3421  1.500
ATOM      6  H6  idaz   1       2.0387   0.6476   0.0000  0.3021  1.200
ATOM      7  H7  idaz   1      -1.4229  -1.7342   0.0000  0.0746  1.200
ATOM      8  H8  idaz   1       1.3451  -1.8164   0.0000  0.2020  1.200
ATOM      9  H9  idaz   1       0.0160   2.1965   0.0000  0.0847  1.200
```

6 F.2.a) primary data for 2-methylimidazole protonated(cation)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
N1         1.4597134446      0.0251955549      1.7239802960
C2         2.1750702878     -0.0404858825      0.5897870250
N3         1.2766610488     -0.0283312652     -0.4089806943
C4        -0.0143104814      0.0439645955      0.0929122640
C5         0.1017545883      0.0776602163      1.4473193208
H6         1.8682605661      0.0359218061      2.6522100001
H7         1.5189943619     -0.0670118466     -1.3932058048
H8        -0.8811637996      0.0660357317     -0.5485573023
H9        -0.6429044811      0.1348312125      2.2254876248
C10        3.6554906748     -0.1282423606      0.4645856260
H11        4.1310462447      0.0426828132      1.4341723994
H12        4.0327576239      0.6234894003     -0.2369514467
H13        3.9573670704     -1.1206929725      0.1090774947
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  N1  idaz   1       1.2695  -0.0276  -0.4410 -0.2850  1.400
ATOM      2  C2  idaz   1       2.1396  -0.0350   0.6199  0.5458  1.500
ATOM      3  N3  idaz   1       1.4843   0.0240   1.7635 -0.5898  1.400
ATOM      4  C4  idaz   1       0.1473   0.0751   1.4288  0.1420  1.500
ATOM      5  C5  idaz   1      -0.0146   0.0442   0.0679 -0.3550  1.500
ATOM      6  H6  idaz   1       1.5199  -0.0608  -1.4188  0.3184  1.200
ATOM      7  H7  idaz   1      -0.6196   0.1339   2.1893  0.0916  1.200
ATOM      8  H8  idaz   1      -0.8852   0.0691  -0.5699  0.2070  1.200
ATOM      9  C9  idaz   1       3.6244  -0.1284   0.4670 -0.4886  2.000
ATOM     10  H10 idaz   1       4.0836   0.0388   1.4436  0.1610  1.200
ATOM     11  H11 idaz   1       4.0147   0.6201  -0.2341  0.1200  1.200
ATOM     12  H12 idaz   1       3.9390  -1.1169   0.1075  0.1325  1.200
```

6 F.2.b) primary data for 2- methylimidazole (neutral)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
N1         1.2694503379     -0.0276354232     -0.4409673072
C2         2.1396083920     -0.0349645849      0.6198613117
N3         1.4843298717      0.0240457004      1.7634939748
C4         0.1473180350      0.0751271627      1.4288152621
C5        -0.0145764169      0.0442325219      0.0679169609
H6         1.5199430962     -0.0608147835     -1.4188454437
H7        -0.6196202816      0.1339006274      2.1892947174
H8        -0.8852002596      0.0691260460     -0.5698988420
C9         3.6244425262     -0.1283586419      0.4670307839
H10        4.0836209590      0.0387609181      1.4436144715
H11        4.0147260610      0.6200582285     -0.2341348647
H12        3.9389948928     -1.1168528052      0.1074642311
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  N1  idaz   1       1.4597   0.0252   1.7240 -0.1958  1.400
ATOM      2  C2  idaz   1       2.1751  -0.0405   0.5898  0.3793  1.500
ATOM      3  N3  idaz   1       1.2767  -0.0283  -0.4090 -0.2083  1.400
ATOM      4  C4  idaz   1      -0.0143   0.0440   0.0929 -0.1253  1.500
ATOM      5  C5  idaz   1       0.1018   0.0777   1.4473 -0.1348  1.500
ATOM      6  H6  idaz   1       1.8683   0.0359   2.6522  0.3623  1.000
ATOM      7  H7  idaz   1       1.5190  -0.0670  -1.3932  0.3674  1.200
ATOM      8  H8  idaz   1      -0.8812   0.0660  -0.5486  0.2356  1.200
ATOM      9  H9  idaz   1      -0.6429   0.1348   2.2255  0.2372  1.200
ATOM     10  C10 idaz   1       3.6555  -0.1282   0.4646 -0.5441  2.000
ATOM     11  H11 idaz   1       4.1310   0.0427   1.4342  0.2029  1.200
ATOM     12  H12 idaz   1       4.0328   0.6235  -0.2370  0.2101  1.200
ATOM     13  H13 idaz   1       3.9574  -1.1207   0.1091  0.2134  1.200
```

6 F.3.a) primary data for 4-methylimidazole protonated(cation)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
N1         1.2932857814      0.8536735542      0.0000000000
C2         0.1498638534      1.5410159032      0.0000000000
N3        -0.8408135870      0.6407885403      0.0000000000
C4        -0.3341121425     -0.6537019286      0.0000000000
C5         1.0279457969     -0.5048324538      0.0000000000
H6         2.2160246768      1.2731263192      0.0000000000
H7         0.0425428444      2.6145129687      0.0000000000
H8        -1.8266655187      0.8763854310      0.0000000000
C9        -1.2010427367     -1.8705861415      0.0000000000
H10       -2.2594975816     -1.6005152044      0.0000000000
H11       -1.0088929924     -2.4830062735     -0.8851778156
H12       -1.0088929924     -2.4830062735      0.8851778156
H13        1.8134228298     -1.2434699880      0.0000000000
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ifreq=1
basis=6-31g**
```

&

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  N1  idaz   1       1.2933   0.8537   0.0000 -0.1583  1.400
ATOM      2  C2  idaz   1       0.1499   1.5410   0.0000  0.0304  1.500
ATOM      3  N3  idaz   1      -0.8408   0.6408   0.0000 -0.2168  1.400
ATOM      4  C4  idaz   1      -0.3341  -0.6537   0.0000  0.2588  1.500
ATOM      5  C5  idaz   1       1.0279  -0.5048   0.0000 -0.2037  1.500
ATOM      6  H6  idaz   1       2.2160   1.2731   0.0000  0.3771  1.000
ATOM      7  H7  idaz   1       0.0425   2.6145   0.0000  0.2307  1.200
ATOM      8  H8  idaz   1      -1.8267   0.8764   0.0000  0.3717  1.200
ATOM      9  C9  idaz   1      -1.2010  -1.8706   0.0000 -0.4711  2.000
ATOM     10  H10 idaz   1      -2.2595  -1.6005   0.0000  0.1709  1.200
ATOM     11  H11 idaz   1      -1.0089  -2.4830  -0.8852  0.1852  1.200
ATOM     12  H12 idaz   1      -1.0089  -2.4830   0.8852  0.1852  1.200
ATOM     13  H13 idaz   1       1.8134  -1.2435   0.0000  0.2397  1.200
```

6 F.3.b) primary data for 4-methylimidazole (neutral)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
N1         1.2855414553      0.8712843681      0.0000000000
C2         0.0766544209      1.5048472849      0.0000000000
N3        -0.9198188543      0.6447014026      0.0000000000
C4        -0.3385465135     -0.6100502930      0.0000000000
C5         1.0323120787     -0.4874586329      0.0000000000
H6         2.1939249080      1.3093964060      0.0000000000
H7        -0.0156725217      2.5820607844      0.0000000000
C8        -1.1790262487     -1.8533524238      0.0000000000
H9        -2.2338614362     -1.5706170458      0.0000000000
H10       -0.9941857010     -2.4752535322     -0.8832235290
H11       -0.9941857010     -2.4752535322      0.8832235290
H12        1.8277073017     -1.2165286368      0.0000000000
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  N1   idaz  1       1.2855   0.8713   0.0000 -0.2896  1.400
ATOM      2  C2   idaz  1       0.0767   1.5048   0.0000  0.2131  1.500
ATOM      3  N3   idaz  1      -0.9198   0.6447   0.0000 -0.5844  1.400
ATOM      4  C4   idaz  1      -0.3385  -0.6101   0.0000  0.4717  1.500
ATOM      5  C5   idaz  1       1.0323  -0.4875   0.0000 -0.3616  1.500
ATOM      6  H6   idaz  1       2.1939   1.3094   0.0000  0.3330  1.200
ATOM      7  H7   idaz  1      -0.0157   2.5821   0.0000  0.0977  1.200
ATOM      8  C8   idaz  1      -1.1790  -1.8534   0.0000 -0.3977  2.000
ATOM      9  H9   idaz  1      -2.2339  -1.5706   0.0000  0.1289  1.200
ATOM     10  H10  idaz  1      -0.9942  -2.4753  -0.8832  0.0967  1.200
ATOM     11  H11  idaz  1      -0.9942  -2.4753   0.8832  0.0967  1.200
ATOM     12  H12  idaz  1       1.8277  -1.2165   0.0000  0.1953  1.200
```

6 F.4.a) primary data for 2- aminoimidazole protonated(cation)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
N1         1.0863440914      0.0477502741      0.0000000000
C2        -0.0393802369     -0.6946448494      0.0000000000
N3        -1.0735304231      0.1710943186      0.0000000000
C4        -0.5917826880      1.4875934215      0.0000000000
C5         0.7557370638      1.4107083313      0.0000000000
H6         2.0277421824     -0.3241027174      0.0000000000
H7        -2.0508017824     -0.0921449436      0.0000000000
H8        -1.2586186559      2.3347775994      0.0000000000
H9         1.5137153062      2.1772289876      0.0000000000
N10       -0.1153882699     -2.0334292141      0.0000000000
H11        0.7147941493     -2.6092915156      0.0000000000
H12       -1.0049066878     -2.5125583148      0.0000000000
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  N1  idaz   1       1.0863   0.0478   0.0000 -0.2933  1.400
ATOM      2  C2  idaz   1      -0.0394  -0.6946   0.0000  0.6505  1.500
ATOM      3  N3  idaz   1      -1.0735   0.1711   0.0000 -0.2930  1.400
ATOM      4  C4  idaz   1      -0.5918   1.4876   0.0000 -0.1502  1.500
ATOM      5  C5  idaz   1       0.7557   1.4107   0.0000 -0.1502  1.500
ATOM      6  H6  idaz   1       2.0277  -0.3241   0.0000  0.3802  1.000
ATOM      7  H7  idaz   1      -2.0508  -0.0921   0.0000  0.3800  1.200
ATOM      8  H8  idaz   1      -1.2586   2.3348   0.0000  0.2449  1.200
ATOM      9  H9  idaz   1       1.5137   2.1772   0.0000  0.2446  1.200
ATOM     10  N10 idaz   1      -0.1154  -2.0334   0.0000 -0.9855  1.400
ATOM     11  H11 idaz   1       0.7148  -2.6093   0.0000  0.4859  1.200
ATOM     12  H12 idaz   1      -1.0049  -2.5126   0.0000  0.4860  1.200
```

6 F.4.b) primary data for 2-aminoimidazole(neutral)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
N1         1.0783692517      0.1745810303      0.0000000000
C2        -0.0138889946     -0.6535562659      0.0000000000
N3        -1.1454063338      0.0212274205      0.0000000000
C4        -0.7654757218      1.3555612337      0.0000000000
C5         0.5921020411      1.4876470782      0.0000000000
H6         2.0485644039     -0.1012688529      0.0000000000
H7        -1.5085085123      2.1415919929      0.0000000000
H8         1.2534780683      2.3401633302      0.0000000000
N9         0.0846576957     -2.0230050234      0.0000000000
H10       -0.7707604465     -2.5527148658      0.0000000000
H11        0.9621041038     -2.5118742036      0.0000000000
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  N1  idaz   1       1.0784   0.1746   0.0000 -0.3266  1.400
ATOM      2  C2  idaz   1      -0.0139  -0.6536   0.0000  0.7814  1.500
ATOM      3  N3  idaz   1      -1.1454   0.0212   0.0000 -0.6306  1.400
ATOM      4  C4  idaz   1      -0.7655   1.3556   0.0000  0.1291  1.500
ATOM      5  C5  idaz   1       0.5921   1.4876   0.0000 -0.4125  1.500
ATOM      6  H6  idaz   1       2.0486  -0.1013   0.0000  0.3311  1.200
ATOM      7  H7  idaz   1      -1.5085   2.1416   0.0000  0.1064  1.200
ATOM      8  H8  idaz   1       1.2535   2.3402   0.0000  0.2218  1.200
ATOM      9  N9  idaz   1       0.0847  -2.0230   0.0000 -1.0975  1.400
ATOM     10  H10 idaz   1      -0.7708  -2.5527   0.0000  0.4612  1.200
ATOM     11  H11 idaz   1       0.9621  -2.5119   0.0000  0.4361  1.200
```

6 F.5.a) primary data for 2-chloroimidazole(cation)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
N1        1.0965850806      0.5589019919      0.0000000000
C2       -0.0055762672     -0.2045487066      0.0000000000
N3       -1.0632165756      0.6199634182      0.0000000000
C4       -0.6269871451      1.9366640169      0.0000000000
C5        0.7341106848      1.8980677824      0.0000000000
H6        2.0435178297      0.1950869034      0.0000000000
H7       -2.0290461840      0.3098610622      0.0000000000
H8       -1.3139495458      2.7679651706      0.0000000000
H9        1.4665801811      2.6895113436      0.0000000000
Cl       -0.0530254393     -1.8896535693      0.0000000000
&
&atomic
atom    basis
Cl      6-31g**
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
```

```
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=1
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  N1  idaz   1       1.0966   0.5589   0.0000 -0.0060  1.400
ATOM      2  C2  idaz   1      -0.0056  -0.2045   0.0000 -0.0001  1.500
ATOM      3  N3  idaz   1      -1.0632   0.6200   0.0000 -0.0060  1.400
ATOM      4  C4  idaz   1      -0.6270   1.9367   0.0000 -0.1382  1.500
ATOM      5  C5  idaz   1       0.7341   1.8981   0.0000 -0.1383  1.500
ATOM      6  H6  idaz   1       2.0435   0.1951   0.0000  0.3224  1.000
ATOM      7  H7  idaz   1      -2.0290   0.3099   0.0000  0.3222  1.200
ATOM      8  H8  idaz   1      -1.3139   2.7680   0.0000  0.2379  1.200
ATOM      9  H9  idaz   1       1.4666   2.6895   0.0000  0.2377  1.200
ATOM     10  Cl  idaz   1      -0.0530  -1.8897   0.0000  0.1684  1.900
```

6 F.5.b) primary data for 2-chloroimidazole(neutral)

jaguar input to estimate the electronic energy

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
basis=cc-pvqz
&
&zmat
N1         1.0679579297      0.6084945010      0.0000000000
C2        -0.0647607453     -0.1529102181      0.0000000000
N3        -1.1612861299      0.5556559902      0.0000000000
C4        -0.7225085432      1.8658845179      0.0000000000
C5         0.6475450538      1.9262993090      0.0000000000
H6         2.0172551729      0.2673687122      0.0000000000
H7        -1.4261345381      2.6856746551      0.0000000000
H8         1.3456974684      2.7484216030      0.0000000000
Cl         0.0295005030     -1.8793595676      0.0000000000
&
```

```
&atomic
atom    basis
Cl      6-31g**
&
```

jaguar input to compute ZPVE and EVE^{298K}

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ifreq=1
basis=6-31g**
&
```

jaguar input to compute the quantum mechnical ESP used as the input for RESP:

```
&gen
iaccg=3
iacscf=2
idft=10001
igeopt=0
molchg=0
multip=1
maxit=150
ip172=2
basis=6-31g**
&
```

pqr-file == input-data for SOLVATE

```
ATOM      1  N1  idaz   1       1.0680   0.6085   0.0000 -0.1741  1.400
ATOM      2  C2  idaz   1      -0.0648  -0.1529   0.0000  0.3210  1.500
ATOM      3  N3  idaz   1      -1.1613   0.5557   0.0000 -0.4678  1.400
ATOM      4  C4  idaz   1      -0.7225   1.8659   0.0000  0.1324  1.500
ATOM      5  C5  idaz   1       0.6475   1.9263   0.0000 -0.3145  1.500
ATOM      6  H6  idaz   1       2.0173   0.2674   0.0000  0.2933  1.200
ATOM      7  H7  idaz   1      -1.4261   2.6857   0.0000  0.0991  1.200
ATOM      8  H8  idaz   1       1.3457   2.7484   0.0000  0.2052  1.200
ATOM      9  Cl  idaz   1       0.0295  -1.8794   0.0000 -0.0945  1.900
```

Additional notes how to reproduce the data given in the tables of this work:

```
idft=10001 [=Beckehalf&half(change to 22111 for B3LYP)]
```

script-file used to start the program SOLVATE:

```
#!/bin/sh

/solvate -ionicstr 0.0 -epsin 1.0 -epsvac 1.0 < name > > solv.out

name.pqr and name.ogm
```

the necessary pqr-files are given in the tables 6a-f (==input data for SOLVATE)
the following ogm-file which specifies the grid was applied for every compound

```
ON_GEOM_CENT 101 1.0
ON_CENT_OF_INTR 101 0.25
```