Towards and Accurate Description of Anharmonic Infrared Spectra in Solution within the Polarizable Continuum Model: Reaction Field, Cavity Field and Nonequilibrium Effects

Chiara Cappelli*

Dipartimento di Chimica e Chimica Industriale,

Università di Pisa,

via Risorgimento, 35 I-56126 Pisa,

Italy; CNR–Consiglio Nazionale delle Ricerche,

Istituto di Chimica dei Composti Organo Metallici (ICCOM-CNR),

UOS di Pisa, Area della Ricerca,

via G. Moruzzi 1, I-56124 Pisa, Italy

Filippo Lipparini and Julien Bloino

Scuola Normale Superiore, Piazza dei Cavalieri, 7 I-56126 Pisa, Italy

Vincenzo Barone

Scuola Normale Superiore,

Piazza dei Cavalieri, 7 I-56126 Pisa,

Italy; CNR–Consiglio Nazionale delle Ricerche,

Istituto di Chimica dei Composti Organo Metallici (ICCOM-CNR), UOS di Pisa,

Area della Ricerca,

via G. Moruzzi 1, I-56124 Pisa, Italy

* Corresponding author: e-mail:chiara@dcci.unipi.it

I. SUPPLEMENTARY MATERIAL

TABLE I. B3LYP/N07Ddiff Calculated Harmonic frequencies (cm^{-1}) of the OH stretching of Phenol in various solvents.

	default		$\alpha = 1.2$		$\alpha = 1.1$		$\alpha = 1.0$	
	ω_{eq}	ω_{neq}	ω_{eq}	ω_{neq}	ν_{eq}	ν_{neq}	ν_{eq}	ν_{neq}
2,2-dimethylbutane	3822.9	3815.2	3822.4	3809.7	3817.4	3791.6	3811.0	3791.6
cyclopentane	3822.1	3813.6	3821.5	3807.4	3816.2	3799.5	3809.2	3787.3
CCl_4	3820.7	3810.7	3819.8	3803.6	3814.0	3794.2	3805.7	3780.0
Tetrachloroethene	3820.5	3810.4	3819.6	3802.9	3813.7	3793.3	3805.3	3778.5
CS_2	3819.1	3807.2	3817.8	3798.5	3811.5	3787.3	3801.8	3770.0
CH_3CN	3806.8	3786.2	3801.4	3769.8	3793.4	3748.2	3774.2	3714.0

TABLE II. B3LYP/N07Ddiff Calculated Harmonic Intensity ratios with respect to 2,2-dimethylbutane of the OH stretching of Phenol in various solvents.

	default		$\alpha = 1.2$		$\alpha = 1.1$		$\alpha = 1.0$	
	I_{eq}	I_{neq}	I_{eq}	I_{neq}	I_{eq}	I_{neq}	I_{eq}	I_{neq}
2,2-dimethylbutane	1	1	1	1	1	1	1	1
cyclopentane	0.978	1.003	0.988	1.011	0.987	1.019	0.997	1.028
CCl_4	0.996	1.035	1.021	1.052	1.021	1.071	1.051	1.093
Tetrachloroethene	0.980	1.037	1.011	1.059	1.006	1.082	1.043	1.110
CS_2	0.964	1.058	1.015	1.095	1.004	1.134	1.066	1.181
CH_3CN	1.535	1.365	1.702	1.448	1.784	1.542	2.020	1.652