Simulation of Vacuum Ultraviolet Absorption Spectra: An Investigation of PIONA Hydrocarbon Class Compounds

Supporting Information

James X. Mao,[†] Phillip Walsh,[‡] Peter Kroll,[†] and Kevin A. Schug[*,†,¶]

[†]*Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington TX, USA*

[‡]*VUV Analytics, Inc., Cedar Park TX, USA*

[¶]*correspondence address: 700 Planetarium Pl., Box 19065, Arlington TX 76019-0065 USA*

E-mail: kschug@uta.edu

Phone: 817-272-3541. Fax: 817-272-3808

Table S1: The optimized FWHMs, scaling factors, and corresponding SSRs for various paraffin compounds.

	Length Form Oscillator Strength			Velocity Form Oscillator Strength		
Paraffin	FWHM	Scaling Factor	SSR	FWHM	Scaling Factor	SSR
Methane	1.2	0.98	1.7	1.2	0.98	1.7
Ethane	1.0	0.98	3.8	1.0	0.98	3.7
Propane	1.1	1.00	4.1	1.1	1.00	4.1
Butane	1.4	1.02	5.4	1.4	1.02	5.5
Pentane	1.4	1.02	9.9	1.3	1.02	9.9
Hexane	1.2	1.02	8.3	1.2	1.02	8.4
Heptane	1.1	1.02	9.4	1.2	1.02	9.3
Octane	1.1	1.02	5.0	1.2	1.02	5.1
Nonane	1.2	1.02	10.8	1.2	1.02	10.7
Decane	1.2	1.02	10.8	1.1	1.02	10.7
Undecane	1.2	1.02	11.5	1.2	1.02	11.5
Dodecane	1.2	1.02	11.7	1.2	1.02	11.7
Tridecane	1.2	1.02	13.0	1.2	1.02	13.0
Tetradecane	1.2	1.02	10.7	1.2	1.02	10.8
Pentadecane	1.2	1.02	12.8	1.2	1.02	12.8
Hexadecane	1.1	1.02	19.0	1.2	1.02	19.0
Heptadecane	1.2	1.02	17.0	1.2	1.02	17.0
Octadecane	1.2	1.02	19.0	1.2	1.02	19.3
Nonadecane	1.1	1.02	22.8	1.1	1.02	22.8
Icosane	1.1	1.02	32.5	1.1	1.02	32.5
Heneicosane	1.1	1.02	25.0	1.1	1.02	25.0
Docosane	1.1	1.02	27.7	1.1	1.02	27.7
Tricosane	1.2	1.02	25.0	1.1	1.02	25.0
Tetracosane	1.1	1.02	29.5	1.1	1.02	29.5
Pentacosane	1.1	1.02	30.5	1.1	1.02	30.7

Table S2: The optimized FWHMs, scaling factors, and corresponding SSRs for various isoparaffin compounds.

	Length Form Oscillator Strength			Velocity Form Oscillator Strength		
Isoparaffin	FWHM	Scaling Factor	SSR	FWHM	Scaling Factor	SSR
2,2-Dimethylbutane	1.9	1.05	1.9	1.3	1.02	2.5
2,3-Dimethylbutane	1.4	1.02	2.5	1.4	1.02	2.9
2,2-Dimethylhexane	1.1	1.02	2.6	1.1	1.02	2.7
2,3-Dimethylhexane	1.0	1.02	1.2	1.0	1.02	1.3
2,4-Dimethylhexane	1.2	1.02	2.7	1.2	1.02	2.8
2,5-Dimethylhexane	1.2	1.02	1.1	1.2	1.02	1.0
3,3-Dimethylhexane	1.1	1.02	5.8	1.1	1.02	6.0
2,2-Dimethylpentane	1.3	1.02	3.7	1.2	1.02	3.8
2,3-Dimethylpentane	1.0	1.00	0.7	0.8	0.99	0.7
2,4-Dimethylpentane	0.9	1.02	10.8	0.9	1.02	11.1
3,3-Dimethylpentane	1.5	1.02	2.0	1.5	1.02	1.9
iso-pentane	1.1	1.01	0.8	1.1	1.01	0.9
iso-butane	1.7	1.01	3.9	1.6	1.01	3.8
iso-octane	1.4	1.02	1.9	1.4	1.02	1.9
2-Methylheptane	1.0	1.02	0.4	1.0	1.02	0.4
2-Methylhexane	1.0	1.02	5.3	0.9	1.02	5.4
2-Methylpentane	1.3	1.02	5.7	1.3	1.02	5.9
3-Methylheptane	1.4	1.02	2.4	1.4	1.02	2.4
3-Methylhexane	1.6	1.02	2.5	1.6	1.02	2.5
3-Methylpentane	1.5	1.02	4.6	1.5	1.02	4.7
4-Methylheptane	1.1	1.02	1.3	1.1	1.02	1.3
3-Ethylpentane	1.2	1.02	5.5	1.2	1.02	5.7
2-Methyl-3-ethylpentane	1.0	1.02	0.9	0.9	1.02	1.0
3-Ethylhexane	0.8	1.02	4.2	0.8	1.02	4.2
2,2-Dimethylpropane	1.7	1.02	4.9	1.7	1.02	5.0
2,2,3-Trimethylbutane	1.5	1.02	1.4	1.4	1.02	1.3
2-Methylnonane	1.2	1.02	11.4	1.2	1.02	11.5
2-Methyloctane	1.1	1.02	9.3	1.1	1.02	10.5
3-Ethyloctane	1.0	1.02	4.7	1.0	1.02	4.8
3-Methylnonane	1.4	1.02	10.8	1.3	1.02	10.6
3-Methyloctane	1.2	1.02	3.9	1.2	1.02	4.0
5-Methylnonane	1.1	1.02	17	1.2	1.02	17.4
2,2-Dimethyloctane	1.3	1.02	6.4	1.1	1.02	6.6
2,3-Dimethyloctane	1.3	1.02	1.8	1.3	1.02	1.8
3,3-Dimethyloctane	1.3	1.02	11.4	1.3	1.02	11.6
3,3-Dimethylheptane	1.0	1.02	1.9	1.0	1.02	2.7
2,5-Dimethylheptane	1.0	1.02	5.3	1.0	1.02	5.9
2,3-Dimethylheptane	1.0	1.02	7.0	1.0	1.02	8.0
3,3-Dimethylpentane	1.4	1.02	5.7	1.4	1.02	6.6
3,4-Dimethylheptane (D)	1.1	1.02	4.4	1.1	1.02	4.4
3,4-Dimethylheptane (L)	1.2	1.02	0.5	1.2	1.02	0.5
2,2,5-Trimethylhexane	1.3	1.02	1.4	1.3	1.02	1.4
2,3,4-Trimethylhexane	1.1	1.02	1.7	1.1	1.02	2.0

Table S3: The optimized FWHMs, scaling factors, and corresponding SSRs for various olefin compounds.

	Length Form Oscillator Strength			Velocity Form Oscillator Strength		
Olefin	FWHM	Scaling Factor	SSR	FWHM	Scaling Factor	SSR
2-Methyl-1-butene	1.2	1.01	13.8	1.2	1.01	13.8
3-Methyl-1-butene	1.0	1.02	27.1	1.0	1.02	27.6
1-Butene	1.0	1.02	35.4	1.1	1.02	36.6
cis-2-Heptene	1.2	1.02	18.3	1.2	1.02	16.3
cis-3-Heptene	1.1	1.02	17.4	1.1	1.02	16.0
trans-2-Heptene	1.1	1.02	9.0	1.1	1.02	8.8
trans-3-Heptene	0.9	1.02	7.0	0.9	1.02	6.1
1-Heptene	1.1	1.02	13.9	1.1	1.02	13.3
1-Hexene	1.2	1.02	12.8	1.2	1.02	12.7
4-Methyl-1-pentene	1.0	1.02	11.0	1.0	1.02	10.4
1-Pentene	1.1	1.01	18.6	1.2	1.01	18.8
2-Methyl-2-pentene	1.1	1.02	10.0	1.2	1.02	10.6
cis-2-Pentene	1.0	1.00	23.6	1.0	1.00	21.8
trans-2-Pentene	1.0	1.02	8.0	1.0	1.02	8.8
2-Methyl-1-pentene	1.2	1.01	9.4	1.2	1.01	9.4
3,3-Dimethyl-1-pentene	0.9	1.01	10.8	0.9	1.01	11.1
3-Methyl-1-pentene	1.3	1.01	24.2	1.4	1.01	24.1
cis-3,4-Dimethyl-2-pentene	0.9	1.02	16.5	0.9	1.02	12.9
cis-4,4-Dimethyl-2-pentene	0.7	0.98	41.2	0.7	0.98	39.2
trans-2-Butene	1.1	1.02	16.2	1.1	1.02	15.4
2-Methyl-2-butene	1.3	1.02	17.1	1.3	1.02	16.4
3,3-Dimethyl-1-butene	1.5	1.02	38.1	1.5	1.02	38.4
cis-2-Butene	1.1	1.02	21.5	1.1	1.02	20.6
cis-4-Methyl-2-pentene	0.7	0.99	32.2	0.7	0.99	27.6
trans-4-Methyl-2-pentene	0.9	0.98	37.5	0.9	0.98	32.6
cis-3-Hexene	1.1	1.00	19.4	1.1	1.00	18.8
cis-2-Hexene	1.1	1.01	18.1	1.1	1.01	15.4
trans-2-Hexene	1.0	1.02	8.0	1.0	1.02	7.8
cis-3-Methyl-3-hexene	0.8	1.00	7.6	0.9	1.00	7.0
trans-3-Hexene	1.1	0.98	8.1	1.1	0.98	8.8
3-Methyl-1-hexene	1.4	1.02	16.8	1.4	1.02	16.2
Ethylene	0.9	1.02	69.8	0.5	1.02	65.1
Propene	1.3	1.02	52.5	1.0	1.01	51.7
Isobutylene	1.5	1.02	52.7	1.5	1.02	52.1
1-Nonene	1.1	1.02	11.3	1.1	1.02	10.7
cis-2-Nonene	1.2	1.02	30.8	1.2	1.02	28.0
cis-3-Nonene	1.0	1.02	16.7	1.1	1.02	15.3
trans-2-Nonene	1.0	1.02	14.5	1.0	1.02	13.8
trans-3-Nonene	0.9	1.02	11.6	0.9	1.02	10.6
1-Decene	1.1	1.02	11.3	1.1	1.02	10.8
1-Octene	1.1	1.02	12.1	1.1	1.02	11.5
cis-2-Octene	1.1	1.02	32.8	1.1	1.02	29.1
trans-2-Octene	1.0	1.02	15.2	1.0	1.02	14.1
1-Dodecene	1.2	1.02	9.7	1.2	1.02	9.2
1-Tetradecene	1.2	1.02	10.8	1.2	1.02	10.5
1-Tridecene	1.2	1.02	10.0	1.2	1.02	9.6
1-Undecene	1.1	1.02	8.5	1.2	1.02	8.0
2,3-Dimethyl-1-butene	0.7	0.99	27.7	0.7	0.99	24.5

Table S4: The optimized FWHMs, scaling factors, and corresponding SSRs for various naphthene compounds.

	Length Form Oscillator Strength			Velocity Form Oscillator Strength		
Naphthene	FWHM	Scaling Factor	SSR	FWHM	Scaling Factor	SSR
1,1-Dimethylcyclopentane	1.3	1.01	1.5	1.4	1.02	1.2
1-Ethyl-1-methylcyclopentane	1.0	1.02	1.9	1.0	1.02	2.5
ccc-1,2,3-Trimethylcyclopentane	1.3	1.02	1.5	1.2	1.02	1.8
cis-1,3-Dimethylcyclopentane	1.3	1.02	7.7	1.4	1.02	9.3
ctc-1,2,3-Trimethylcyclopentane	1.4	1.02	8.1	1.4	1.02	8.4
ctc-1,2,4-Trimethylcyclopentane	1.3	1.02	12.7	1.3	1.02	13.6
ctt-1,2,4-Trimethylcyclopentane	1.7	1.02	5.4	1.7	1.02	5.4
Cyclopentane	1.5	1.01	1.2	1.6	1.02	1.3
Ethylcyclopentane	1.5	1.01	1.5	1.5	1.01	1.5
Isopropylcyclopentane	1.0	1.02	13.6	1.3	1.02	15.8
Methylcyclopentane	1.2	1.02	1.2	1.1	1.02	2.0
n-Propylcyclopentane	1.0	1.01	2.9	1.1	1.02	3.4
trans-1,2-Dimethylcyclopentane	1.4	1.02	1.1	1.4	1.02	1.6
trans-1,3-Dimethylcyclopentane	1.4	1.02	12.1	1.5	1.02	14.9
cis-1,2-Dimethylcyclopentane	1.0	1.00	0.3	1.0	1.01	0.2
Methylcyclohexane	1.3	1.02	2.5	1.4	1.02	2.7
cis-1,2-Dimethylcyclohexane	1.2	1.02	1.9	1.2	1.02	2.0
Cyclohexane	1.9	1.02	5.8	1.9	1.02	6.2
trans-1,2-Dimethylcyclohexane	1.0	1.02	1.1	1.0	1.02	1.1
trans-1,4-Dimethylcyclohexane	1.2	1.02	2.5	1.2	1.02	2.5
1,1-Dimethylcyclohexane	1.0	1.02	3.1	1.0	1.02	3.1
cis-1,4-Dimethylcyclohexane	1.3	1.02	1.8	1.2	1.02	1.8
Cyclopropane	1.2	1.02	2.9	1.2	1.02	2.9
ctc-1,2,3-Trimethylcyclohexane	1.0	1.02	1.7	1.0	1.02	1.8
ccc-1,3,5-Trimethylcyclohexane	1.3	1.02	17.7	1.2	1.02	18.0
1,1,2-Trimethylcyclohexane	1.2	1.02	1.3	1.2	1.02	1.2
1,1,4-Trimethylcyclohexane	1.2	1.02	2.8	1.2	1.02	2.7
ctc-1,2,4-Trimethylcyclohexane	1.3	1.02	0.8	1.3	1.02	0.7
ctt-1,2,4-Trimethylcyclohexane	1.1	1.02	0.7	1.1	1.02	0.8
Isobutylcyclohexane	1.4	1.02	3.4	1.4	1.02	3.4
Isobutylcyclopentane	1.3	1.02	0.4	1.2	1.02	0.4
Isopropylcyclohexane	1.9	1.02	1.9	1.9	1.02	1.8
n-Butylcyclopentane	1.0	1.02	0.5	1.0	1.02	0.8
t-1-Methyl-2-propylcyclohexane	1.0	1.02	1.0	1.0	1.02	1.1
t-1-Methyl-2-(4MP)cyclopentane	1.0	1.02	3.6	1.0	1.02	4.5

Table S5: The optimized FWHMs, scaling factors, and corresponding SSRs for various aromatic compounds.

	Length Form Oscillator Strength			Velocity Form Oscillator Strength		
Aromatic	FWHM	Scaling Factor	SSR	FWHM	Scaling Factor	SSR
Benzene	0.4	1.00	12.4	0.4	1.00	12.1
Toluene	0.5	1.01	12.7	0.5	1.01	12.3
Ethylbenzene	0.4	1.00	10.0	0.4	1.00	9.8
n-Propylbenzene	0.4	1.00	9.4	0.4	1.00	9.1
Isopropylbenzene	0.5	1.00	11.9	0.5	1.00	11.6
m-Xylene	0.5	1.01	12.1	0.5	1.01	11.8
p-Xylene	0.5	1.01	11.0	0.5	1.01	10.8
o-Xylene	0.5	1.00	11.5	0.5	1.00	11.7
1-Methyl-2-ethylbenzene	0.5	1.00	14.7	0.5	1.00	14.5
1-Methyl-3-ethylbenzene	0.4	1.01	10.2	0.4	1.01	10.2
1-Methyl-4-ethylbenzene	0.5	1.01	8.4	0.5	1.01	8.5
1,2,4-Triethylbenzene	0.5	0.99	13.5	0.5	0.99	13.9
1,3,5-Triethylbenzene	0.3	0.98	89.4	0.3	0.98	85.3
1,2,4-Trimethylbenzene	0.5	1.01	10.8	0.5	1.01	10.7
1,3,5-Trimethylbenzene	0.4	1.01	19.4	0.4	1.01	19.3
1-Methyl-2-isopropylbenzene	0.5	1.01	11.8	0.5	1.01	11.7
1-Methyl-3-isopropylbenzene	0.5	1.01	15.0	0.5	1.01	15.2
1-Methyl-4-isopropylbenzene	0.5	1.01	7.5	0.5	1.01	7.2
1-Methyl-2-n-propylbenzene	0.5	1.00	11.1	0.5	1.00	11.3
1-Methyl-3-n-propylbenzene	0.5	1.01	13.5	0.5	1.01	13.8
1-Methyl-4-n-propylbenzene	0.5	1.01	7.8	0.5	1.01	8.2
tert-1-Butyl-2-methylbenzene	0.5	1.01	11.2	0.5	1.01	11.0
1,2-Dimethyl-3-ethylbenzene	0.5	1.00	9.0	0.5	1.00	9.3
1,2-Dimethyl-4-ethylbenzene	0.5	1.00	12.3	0.5	1.00	13.2
1,3-Dimethyl-2-ethylbenzene	0.4	1.00	12.4	0.4	1.00	12.4
1,3-Dimethyl-5-ethylbenzene	0.4	1.01	17.6	0.4	1.01	17.3
1,4-Dimethyl-2-ethylbenzene	0.6	1.00	11.3	0.5	1.00	11.5
1,3-Dimethyl-4-ethylbenzene	0.5	1.01	5.2	0.5	1.01	5.2
n-Butylbenzene	0.5	1.00	15.9	0.5	1.00	16.0
n-Hexylbenzene	0.5	1.00	16.8	0.5	1.00	16.8
n-Pentylbenzene	0.4	1.00	15.1	0.4	1.00	15.2
Isobutylbenzene	0.4	1.00	12.8	0.4	1.00	12.3
sec-Butylbenzene	0.4	1.00	11.4	0.4	1.00	10.9
tert-Butylbenzene	0.5	1.00	13.9	0.4	1.00	13.5
1,2,3,5-Tetramethylbenzene	0.6	1.02	15.2	0.6	1.02	15.1
1,2,4,5-Tetramethylbenzene	0.6	1.02	11.5	0.6	1.02	11.9
1,2-Diethylbenzene	0.4	1.00	12.7	0.4	1.00	12.7
tert-1-Butyl-3,4,5-trimethylbenzene	0.5	1.00	15.0	0.5	1.01	15.5
Pentamethylbenzene	0.6	1.01	12.8	0.6	1.02	12.8
2-Methylbutylbenzene	0.4	1.00	10.0	0.4	1.00	9.7
t-1-Butyl-3,5-dimethylbenzene	0.5	1.01	16.5	0.5	1.01	16.8
t-1-Butyl-4-ethylbenzene	0.5	1.00	7.0	0.5	1.00	7.1