Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for: Core-Excited and Shape Resonances of Uracil

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Table 1: Complex energies of the first three A" shape resonances associated with Analytic Continuation using the EOM-EA-CCSD/6-31+G(d) stabilization graph (Figure 5 (top panel)). Results for each avoided crossing (X *i*) are shown.

	GPA	$1\pi^*$ $E_r + \Gamma$ [eV]	$2\pi^*$ $E_r + \Gamma$ [eV]	$3\pi^*$ $E_r + \Gamma$ [eV]
	(3,3,3)	0.9384 (0.0000)	2.6144 (0.1157)	5.6423 (0.0531)
	(4,4,4)	0.9384 (0.0000)	2.6110 (0.1179)	5.6425 (0.0504)
X1	(5,5,5)	0.9372 (0.0003)	2.6113 (0.1183)	5.6453 (0.0503)
	(3,3,3)		2.5697 (0.0674)	5.8407 (0.0645)
	(4,4,4)		2.6061 (0.1070)	5.8406 (0.0638)
X2	(5,5,5)		2.6104 (0.1074)	5.8403 (0.0636)
	(3,3,3)			5.6995 (0.4649)
	(4,4,4)			5.7009 (0.4702)
X3	(5,5,5)			5.6827 (0.4439)
	(3,3,3)			5.2828 (0.2067)
	(4,4,4)			5.2819 (0.2055)
X4	(5,5,5)			5.2810 (0.1982)

Table 2: Complex energies of the first three $A^{''}$ shape resonances associated with Analytic Continuation using the EOM-EA-CCSD/6-311+G(d) stabilization graph (Figure 5 (middle panel)). Results for each avoided crossing (X *i*) are shown.

	GPA	$1\pi^*$ $E_r + \Gamma$ [eV]	$2\pi^*$ $E_r + \Gamma$ [eV]	$3\pi^*$ $E_r + \Gamma$ [eV]
	(3,3,3)	1.0015 (0.0000)	2.5152 (0.1226)	5.4608 (0.0253)
	(4,4,4)	1.0025 (0.0000)	2.4949 (0.1136)	5.4613 (0.0223)
X1	(5,5,5)	1.0011 (0.0003)	2.4953 (0.1132)	5.4660 (0.0272)
	(3,3,3)		2.4744 (0.0876)	5.6301 (0.0632)
	(4,4,4)		2.4397 (0.0982)	5.6305 (0.0637)
X2	(5,5,5)		2.5076 (0.0963)	5.6333 (0.0619)
	(3,3,3)			5.5844 (0.4186)
	(4,4,4)			5.5833 (0.4144)
X3	(5,5,5)			5.5837 (0.4065)
	(3,3,3)			5.1747 (0.2975)
	(4,4,4)			5.1752 (0.3010)
X4	(5,5,5)			5.1812 (0.2927)

Table 3: Complex energies of the first three A^{1} shape resonances associated with Analytic Continuation using the EOM-EA-CCSD/aug-cc-pVDZ stabilization graph (Figure 5 (bottom panel)). Results for each avoided crossing (X *i*) are shown.

		1π*	2π*	3π*
	GPA	$E_r + \Gamma$ [eV]	$E_r + \Gamma$ [eV]	$E_r + \Gamma$ [eV]
	(3,3,3)	0.7444 (0.0077)	2.3435 (0.0338)	4.8249 (0.1056)
	(4,4,4)	0.7749 (0.0276)	2.3484 (0.0539)	4.8274 (0.1050)
X1	(5,5,5)	0.7725 (0.0307)	2.3508 (0.0458)	4.8278 (0.1053)
	(3,3,3)		-	5.2683 (0.1192)
	(4,4,4)		2.3943 (0.1029)	5.2683 (0.1192)
X2	(5,5,5)		2.3975 (0.1103)	5.2764 (0.1218)
	(3,3,3)			5.2123 (0.4450)
	(4,4,4)			5.2188 (0.4390)
X3	(5,5,5)			5.3979 (0.4492)
	(3,3,3)			4.9417 (0.2409)
	(4,4,4)			4.9425 (0.2384)
X4	(5,5,5)			4.9057 (0.2162)

Table 4: $\pi^1(\pi^*)^2$ core-excited resonance energies and widths (in parenthesis) in eV for the 6-31+G(d), 6-311+G(d), aug-cc-pVDZ and aug-cc-pVDZ+1s,1p,1d scaled basis functions.

GPA	6-31+G(d)	6-311+G(d)	aug-cc-pVDZ	aug-cc-pVDZ+1s,1p,1d
(3,3,3)	5.6622 (0.0936)	5.5608 (0.1012)	5.3240 (0.0877)	5.2987 (0.1034)
(4,4,4)	5.6626 (0.0934)	5.5620 (0.1012)	5.3248 (0.0875)	5.2979 (0.1033)
(5,5,5)	5.6627 (0.0932)	5.5612 (0.1007)	5.3259 (0.0866)	5.2531 (0.1686)

Table 5: $n^1(\pi^*)^2$ core-excited resonance energies and widths (in parenthesis) in eV for the 6-31+G(d) and 6-311+G(d) basis functions.

GPA	6-31+Gd	6-311+Gd
(3,3,3)	6.5385 (0.0126)	6.2971 (0.0365)
(4,4,4)	6.5424 (0.0363)	6.3006 (0.0365)
(5,5,5)	6.5398 (0.0370)	6.3046 (0.0410)

Table 6: Energies and widths obtained at the CASSCF/6-31+G(d) and XMCQDPT2/6-31+G(d) levels. The energy of the first resonance has been shifted to the experimental value of 0.22 eV. Both the analytic continuation for branch and stationary points are given due to the vanishingly small widths obtained when determining widths via stationary points.

		MCSCF		XMCQDPT	
		Branch Point	Stationary Point	Branch Point	Stationary Point
	GPA	$E_r + \Gamma$	$E_r + \Gamma$	$E_r + \Gamma$	$E_r + \Gamma$
	(3,3,3)	0.22 (0.1133)	0.22 (0.0000)	0.22 (0.0043)	0.22 (0.0000)
	(4,4,4)	0.22 (0.1164)	0.22 (0.0000)	0.22 (0.0038)	0.22 (0.0000)
	(5,5,5)	0.22 (0.1173)	0.22 (0.0000)	0.22 (0.0061)	0.22 (0.0000)
$1\pi^*$	(3,3,3,3)	0.22 (0.1203)	-	0.22 (0.0035)	-
	(3,3,3)	1.8887 (0.0477)	1.8090 (0.0000)	1.1863 (0.0156)	1.0763 (0.0000)
	(4,4,4)	1.9023 (0.0467)	1.7945 (0.0056)	1.1865 (0.0157)	1.0428 (0.0000)
	(5,5,5)	1.8987 (0.0475)	1.7967 (0.0064)	1.1861 (0.0172)	1.0778 (0.0000)
$2\pi^*$	(3,3,3,3)	1.8883 (0.0463)	-	1.1865 (0.0157)	-
	(3,3,3)	4.8483 (0.0951)	4.8146 (0.0000)	4.1756 (0.0105)	3.9831 (0.0000)
	(4,4,4)	4.8479 (0.0953)	4.8149 (0.0000)	4.1775 (0.0102)	3.9802 (0.0000)
	(5,5,5)	4.8564 (0.0954)	4.7710 (0.0036)	4.1749 (0.0114)	3.9845 (0.0000)
$3\pi^*+\pi(\pi^*)^2$	(3,3,3,3)	-	-	4.1756 (0.0119)	-
	(3,3,3)	5.5961 (0.3038)	5.6892 (0.1253)	4.5561 (0.0883)	4.6267 (0.0000)
	(4,4,4)	5.6076 (0.3145)	5.4159 (0.1708)	4.5551 (0.0876)	4.6267 (0.0000)
$\pi(\pi^*)^2$	(5,5,5)	5.5733 (0.2995)	5.5107 (0.1171)	4.5546 (0.0876)	4.6267 (0.0000)
$+3\pi^*$	(3,3,3,3)	5.6250 (0.2836)	-	4.5571 (0.0850)	