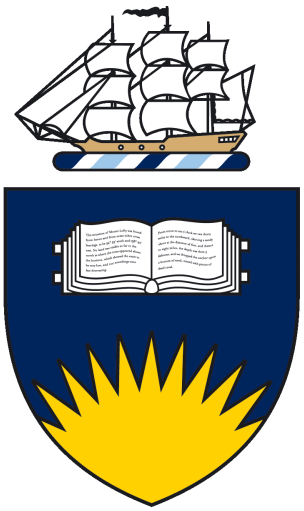

Flinders
UNIVERSITY

Dynamical (e,2e) Studies of Bio-Molecules

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The central activity of engineering, as distinguished from science, is the design of new devices, processes and systems.

$\sim$ Myron T. Tribus (1921-)

A

Appendix A: Experimental Data

A.1 Pyrimidine

Parameter (Orbital)	Values	Error
Height ($7b_2$)	1.34	$\pm$ 0.62
Centre (eV) ($7b_2$)	9.84	$\pm$ 0.27
HWHM (eV) ($7b_2$)	0.55	$\pm$ 0.07
Height ($11a_1$)	1.38	$\pm$ 346.9
Centre (eV) ($11a_1$)	11.14	$\pm$ 14.75
HWHM (eV) ($11a_1$)	0.55	$\pm$ 0.07
Height ($1a_2$)	0.40	$\pm$ 0.31
Centre (eV) ($1a_2$)	12.62	$\pm$ 0.71
HWHM (eV) ($1a_2$)	0.55	$\pm$ 0.07
Height ($10a_1$)	2.80	$\pm$ 0.29
Centre (eV) ($10a_1$)	13.94	$\pm$ 0.08
HWHM (eV) ($10a_1$)	0.55	$\pm$ 0.07
Height ($6b_2$)	1.03	$\pm$ 0.28
Centre (eV) ($6b_2$)	15.29	$\pm$ 0.18
HWHM (eV) ($6b_2$)	0.55	$\pm$ 0.07
Height ($9a_1$)	1.00	$\pm$ 0.60
Centre (eV) ($9a_1$)	16.88	$\pm$ 0.32
HWHM (eV) ($9a_1$)	0.55	$\pm$ 0.07
Height ($5b_2$)	2.26	$\pm$ 0.51
Centre (eV) ($5b_2$)	17.73	$\pm$ 0.17
HWHM (eV) ($5b_2$)	0.55	$\pm$ 0.07
Height ($8a_1$)	0.67	$\pm$ 0.26
Centre (eV) ($8a_1$)	19.08	$\pm$ 0.27
HWHM (eV) ($8a_1$)	0.55	$\pm$ 0.07
Height ($7a_1$)	0.43	$\pm$ 0.22
Centre (eV) ($7a_1$)	20.90	$\pm$ 0.44
HWHM (eV) ($7a_1$)	0.55	$\pm$ 0.07

Table A.1: *Fitting Data for the pyrimidine binding energy spectrum, shown in Figure 4.2.*

θ_{ej} (degrees)	Intensity (arb. units)	Error
55	0.836	±0.103
60	0.681	±0.100
65	0.735	±0.099
70	0.624	±0.096
75	0.610	±0.094
80	1	±0.098
85	0.822	±0.098
90	0.916	±0.098
95	0.866	±0.097
100	0.507	±0.094
105	0.529	±0.093
110	0.500	±0.091
115	0.313	±0.089
120	0.175	±0.072
240	0.076	±0.083
245	0.109	±0.083
250	0.057	±0.081
255	0.133	±0.081
260	0.079	±0.080
265	0.215	±0.081
270	-0.004	±0.078
275	0.166	±0.078

Table A.2: *Experimental data for the* $7b_2$ *orbital of pyrimidine, after normalisation.* $\theta_{sc} = -15°$, $E_0 = 250$ *eV and* $E_{ej} = 20$ *eV.*

θ_{ej} (degrees)	Intensity (arb. units)	Error
65	0.912	±0.118
70	0.739	±0.115
75	0.804	±0.117
80	1	±0.121
85	0.841	±0.114
90	0.755	±0.112
95	0.977	±0.114
100	0.682	±0.108
105	0.701	±0.106
110	0.687	±0.104
115	0.445	±0.101
120	0.571	±0.101
240	0.392	±0.073
245	0.500	±0.075
250	0.449	±0.075
255	0.257	±0.073
260	0.294	±0.075
265	0.414	±0.078
270	0.455	±0.079
275	0.449	±0.079
280	0.268	±0.079
285	0.236	±0.078

Table A.3: *Experimental data for the* $10a_1$ *orbital of pyrimidine, after normalisation.* $\theta_{sc} = -5°$, $E_0 = 250$ *eV and* $E_{ej} = 20$ *eV.*

θ_{ej} (degrees)	Intensity (arb. units)	Error
60	0.992	±0.106
65	0.995	±0.107
70	1.007	±0.105
75	1	±0.106
80	0.905	±0.108
85	0.808	±0.105
90	0.532	±0.103
95	0.609	±0.106
100	0.618	±0.109
105	0.310	±0.107
110	0.243	±0.107
115	0.246	±0.109
120	0.200	±0.111
240	0.185	±0.065
245	0.016	±0.065
250	0.020	±0.065
255	0.150	±0.065
260	0.213	±0.066
265	0.149	±0.067
270	0.169	±0.068
275	0.212	±0.067
280	0.012	±0.069

Table A.4: *Experimental data for the* $10a_1$ *orbital of pyrimidine, after normalisation.* $\theta_{sc} = -10°$, $E_0 = 250$ *eV and* $E_{ej} = 20$ *eV.*

θ_{ej} (degrees)	Intensity (arb. units)	Error
55	0.980	±0.074
60	0.751	±0.072
65	0.819	±0.071
70	0.833	±0.070
75	1	±0.071
80	0.977	±0.070
85	0.878	±0.070
90	0.773	±0.071
95	0.730	±0.072
100	0.348	±0.071
105	0.330	±0.071
110	0.134	±0.071
115	0.194	±0.072
120	0.184	±0.072
240	0.095	±0.079
245	0.132	±0.079
250	0.202	±0.078
255	-0.041	±0.075
260	0.147	±0.075
265	0.102	±0.074
270	0.107	±0.072
275	0.060	±0.070

Table A.5: *Experimental data for the* $10a_1$ *orbital of pyrimidine, after normalisation.* $\theta_{sc} = -15°$, $E_0 = 250$ *eV and* $E_{ej} = 20$ *eV.*

A.2 α-Tetrahydrofurfuryl Alcohol

Parameter (Orbital)	Values	Error
Height (28a)	90.40	± 20.81
Centre (eV) (28a)	9.88	± 0.14
HWHM (eV) (28a)	0.45	± 0
Height (27a)	154.22	± 46.83
Centre (eV) (27a)	10.86	± 0.09
HWHM (eV) (27a)	0.4	± 0

Table A.6: *Fitting Data for the tetrahydrofurfuryl alcohol binding energy spectrum, shown in Figure 5.2. It is worth noting that there are only two Gaussians listed above. This is because there is insufficent data to provide an accurate Gaussian fit on the third orbital.*

θ_{ej} (degrees)	Intensity (arb. units)	Error
65	1.55	±0.21
70	1.37	±0.21
75	1.28	±0.21
80	1.39	±0.21
85	1.49	±0.21
90	1.51	±0.21
95	1.45	±0.21
100	1.26	±0.20
105	1.22	±0.20
110	0.79	±0.19
115	0.68	±0.19
120	0.79	±0.19
240	0.75	±0.16
245	1.01	±0.16
250	0.94	±0.16
255	1.06	±0.17
260	1.02	±0.17
265	0.72	±0.17
270	0.85	±0.17
275	0.79	±0.17
280	1.04	±0.18
285	0.73	±0.17

Table A.7: *Experimental data for the* 28*a (HOMO) orbital of THFA, after normalisation.* $\theta_{sc} = -5°$, $E_0 = 250$ *eV and* $E_{ej} = 20$ *eV.*

θ_{ej} (degrees)	Intensity (arb. units)	Error
60	1.14	±0.23
65	0.78	±0.22
70	0.65	±0.21
75	1.02	±0.21
80	0.79	±0.21
85	1.23	±0.21
90	1.36	±0.21
95	1.07	±0.21
100	1.28	±0.21
105	0.79	±0.20
110	1.02	±0.20
115	0.50	±0.20
120	0.82	±0.20
240	0.19	±0.21
245	0.19	±0.21
250	0.29	±0.21
255	0.59	±0.22
260	0.13	±0.22
265	0.42	±0.23
270	0.21	±0.23
275	0.00	±0.24
280	0.34	±0.25

Table A.8: *Experimental data for the* 28*a (HOMO) orbital of THFA, after normalisation.* $\theta_{sc} = -10°$, $E_0 = 250$ *eV and* $E_{ej} = 20$ *eV.*

θ_{ej} (degrees)	Intensity (arb. units)	Error
55	0.96	±0.33
60	1.07	±0.32
65	0.92	±0.31
70	1.80	±0.29
75	1.28	±0.27
80	1.39	±0.27
85	1.40	±0.26
90	1.38	±0.26
95	1.49	±0.26
100	1.58	±0.26
105	1.13	±0.25
110	1.41	±0.25
115	1.40	±0.26
120	0.90	±0.26
240	0.26	±0.20
245	0.41	±0.21
250	0.32	±0.21
255	0.16	±0.22
260	0.55	±0.23
265	0.00	±0.23
270	0.53	±0.24
275	0.22	±0.25

Table A.9: *Experimental data for the* 28*a (HOMO) orbital of THFA, after normalisation.* $\theta_{sc} = -15^{\circ}$, $E_0 = 250\ eV$ *and* $E_{ej} = 20\ eV$.

A.3 Tetrahydrofuran

Parameter (Orbital)	Values	Error
Height $(9b + 12a')$	0.745	$\pm$0.35
Centre (eV) $(9b + 12a')$	9.76	$\pm$1.85
HWHM (eV) $(9b + 12a')$	0.63	$\pm$ 0.32
Height $(11a + 11a' + 8a'')$	1.04	$\pm$0.58
Centre (eV) $(11a + 11a' + 8a'')$	11.32	$\pm$1.84
HWHM (eV) $(11a + 11a' + 8a'')$	0.63	$\pm$ 0.32
Height $(10a + 10' + 8b + 7a'' + 9a)$	2.35	$\pm$1.14
Centre (eV) $(10a + 10' + 8b + 7a'' + 9a)$	12.42	$\pm$1.84
HWHM (eV) $(10a + 10' + 8b + 7a'' + 9a)$	0.63	$\pm$ 0.32
Height $(6a'' + 7b + 9a' + 6b + 8a)$	1.51	$\pm$0.78
Centre (eV) $(6a'' + 7b + 9a' + 6b + 8a)$	13.87	$\pm$1.84
HWHM (eV) $(6a'' + 7b + 9a' + 6b + 8a)$	0.63	$\pm$ 0.32
Height $(5a'' + 8a'' + 7a)$	1.76	$\pm$0.90
Centre (eV) $(5a'' + 8a'' + 7a)$	15.42	$\pm$1.84
HWHM (eV) $(5a'' + 8a'' + 7a)$	0.63	$\pm$ 0.32
Height $(5b + 7a')$	2.11	$\pm$1.13
Centre (eV) $(5b + 7a')$	17.00	$\pm$1.84
HWHM (eV) $(5b + 7a')$	0.63	$\pm$ 0.32
Height $(6a + 6a')$	1	$\pm$0
Centre (eV) $(6a + 6a')$	18.84	$\pm$1.84
HWHM (eV) $(6a + 6a')$	0.63	$\pm$ 0.32

Table A.10: *Fitting Data for the tetrahydrofuran binding energy spectrum, shown in Figure 6.2. It is worth noting that the HWHM for THF is larger than the other molecules - this is to provide the best visual fit to the available data.*

θ_{ej} (degrees)	Intensity (arb. units)	Error
65	2.40	±0.52
70	3.21	±0.52
75	1.71	±0.50
80	1.79	±0.54
85	1.88	±0.54
90	1.53	±0.51
95	1.30	±0.50
100	1.69	±0.48
105	1.98	±0.47
110	1.39	±0.45
115	1.54	±0.44
120	0.86	±0.42
240	0.67	±0.30
245	0.97	±0.31
250	1.29	±0.32
255	0.71	±0.33
260	0.40	±0.33
265	0.51	±0.34
270	1.12	±0.36
275	0.45	±0.36
280	0.21	±0.37
285	0.78	±0.35

Table A.11: *Experimental data for the* $9b + 12a'$ *(HOMO) orbital of THF, after normalisation.* $\theta_{sc} = -5°$, $E_0 = 250\ eV$ *and* $E_{ej} = 20\ eV$.

A.4 Tetrahydropyran

Parameter (Orbital)	Values	Error
Height ($15a'$)	53.60	$\pm$17.92
Centre (eV) ($15a'$)	9.28	$\pm$0.54
HWHM (eV) ($15a'$)	0.55	$\pm$ 0
Height ($14a' + 9a'$)	150.14	$\pm$20.41
Centre (eV) ($14a' + 9a'$)	11.33	$\pm$0.51
HWHM (eV) ($14a' + 9a'$)	0.55	$\pm$ 0
Height ($13a' + 8a''$)	154.73	$\pm$25.6
Centre (eV) ($13a' + 8a''$)	12.60	$\pm$0.51
HWHM (eV) ($13a' + 8a''$)	0.55	$\pm$ 0
Height ($12a' + 7a'' + 6a''$)	201.91	$\pm$26.91
Centre (eV) ($12a' + 7a'' + 6a''$)	13.66	$\pm$0.49
HWHM (eV) ($12a' + 7a'' + 6a''$)	0.55	$\pm$ 0
Height ($11a' + 10a' + 5a''$)	227.29	$\pm$20
Centre (eV) ($11a' + 10a' + 5a''$)	15.29	$\pm$0.51
HWHM (eV) ($11a' + 10a' + 5a''$)	0.55	$\pm$ 0
Height ($9a'$)	149.60	$\pm$18.68
Centre (eV) ($9a'$)	16.70	$\pm$0.53
HWHM (eV) ($9a'$)	0.55	$\pm$ 0

Table A.12: *Fitting Data for the tetrahydropyran binding energy spectrum, shown in Figure 6.3.*

θ_{ej} (degrees)	Intensity (arb. units)	Error
60	0.97	±0.28
65	1.19	±0.21
70	1.40	±0.19
75	1.05	±0.19
80	1.09	±0.21
85	1.09	±0.19
90	1.19	±0.19
95	0.77	±0.19
100	0.93	±0.16
105	0.93	±0.16
110	0.95	±0.16
115	0.74	±0.14
120	0.91	±0.14
240	0.37	±0.19
245	1.23	±0.21
250	0.91	±0.21
255	0.67	±0.21
260	0.56	±0.21
265	1.05	±0.21
270	0.19	±0.21
275	0.93	±0.23
280	0.74	±0.21
285	0.51	±0.21

Table A.13: *Experimental data for the* $15a'$ *(HOMO) orbital of THP, after normalisation.* $\theta_{sc} = -5^{\circ}$, $E_0 = 250\ eV$ *and* $E_{ej} = 20\ eV$.

A.5 1,4 - Dioxane

Parameter (Orbital)	Values	Error
Height ($8a_g$)	0.32	±0.13
Centre (eV) ($8a_g$)	9.38	±0.10
HWHM (eV) ($8a_g$)	0.55	±0
Height ($7a_g$)	0.65	±0.24
Centre (eV) ($7a_g$)	10.68	±0.10
HWHM (eV) ($7a_g$)	0.55	±0
Height ($7b_u$)	0.55	±0.24
Centre (eV) ($7b_u$)	11.21	±0.10
HWHM (eV) ($7b_u$)	0.55	±0
Height ($5a_u$)	0.819	±0.18
Centre (eV) ($5a_u$)	12.58	±0.10
HWHM (eV) ($5a_u$)	0.55	±0
Height ($4b_g + 6b_u$)	0.86	±0.18
Centre (eV) ($4b_g + 6b_u$)	13.35	±0.10
HWHM (eV) ($4b_g + 6b_u$)	0.55	±0
Height ($4a_u$)	0.94	±0.19
Centre (eV) ($4a_u$)	14.06	±0.10
HWHM (eV) ($4a_u$)	0.55	±0
Height ($6a_g$)	0.70	±0.18
Centre (eV) ($6a_g$)	15.38	±0.10
HWHM (eV) ($6a_g$)	0.55	±0
Height ($3a_u + 3b_g$)	1.21	±0.18
Centre (eV) ($3a_u + 3b_g$)	16.11	±0.10
HWHM (eV) ($3a_u + 3b_g$)	0.55	±0
Height ($5b_u + 5a_g$)	1.25	±0.20
Centre (eV) ($5b_u + 5a_g$)	17.01	±0.10
HWHM (eV) ($5b_u + 5a_g$)	0.55	±0

Table A.14: *Fitting Data for the 1,4-dioxane binding energy spectrum, shown in Figure 6.4.*

θ_{ej} (degrees)	Intensity (arb. units)	Error
65	0.59	±0.14
70	0.50	±0.13
75	0.53	±0.13
80	0.53	±0.14
85	0.35	±0.13
90	0.45	±0.13
95	0.38	±0.12
100	0.574	±0.12
105	0.34	±0.11
110	0.42	±0.11
115	0.38	±0.10
120	0.40	±0.10
285	0.20	±0.11
280	0.20	±0.11
275	0.23	±0.11
270	0.35	±0.11
265	0.43	±0.11
260	0.52	±0.10
255	0.39	±0.10
250	0.23	±0.10
245	0.28	±0.10
240	0.26	±0.09

Table A.15: *Experimental data for the $8a_g$ (HOMO) orbital of 1,4-dioxane, after normalisation. $\theta_{sc} = -5^\circ$, $E_0 = 250\ eV$ and $E_{ej} = 20\ eV$.*