

Supplementary Informations

In the following, t refers to the number of the transition computed, λ to the transition wavelength (nm) and f to the oscillator strength associated to the t^{th} transition, $\tilde{\chi}_{\omega}$ are in atomic units of charge, $\tilde{\zeta}_{\pm}$ and ζ are given in Å.

PBE0 - vacuum

#	t	λ	f	$\tilde{\chi}_{-}$	$\tilde{\chi}_{+}$	$\tilde{\zeta}_{\pm}$	ζ	ϕ_S
I-a	1	240.47	0.2748	0.57	0.56	1.26	0.69	0.75
I-b	1	254.15	0.4204	0.58	0.57	0.84	0.47	0.72
1II-a	1	293.71	0.8110	0.54	0.54	0.03	0.01	0.76
2II-a	1	337.59	1.2869	0.54	0.54	1.67	0.81	0.79
3II-a	1	394.25	1.7290	0.56	0.56	2.96	1.49	0.76
4II-a	1	440.81	2.0936	0.59	0.59	4.44	2.24	0.78
5II-a	1	485.82	2.4037	0.62	0.61	5.88	3.05	0.78
1II-b	1	309.94	0.9267	0.55	0.56	0.32	0.15	0.77
2II-b	1	355.17	1.4236	0.56	0.56	1.89	0.94	0.79
3II-b	1	412.33	1.8711	0.58	0.58	3.03	1.59	0.75
4II-b	1	459.54	2.2402	0.60	0.60	4.47	2.41	0.75
5II-b	1	505.23	2.5505	0.62	0.63	5.74	3.25	0.73
1III-a	2	293.97	0.0285	0.89	0.88	0.76	0.68	0.30
2III-a	2	323.81	0.1442	0.85	0.85	0.01	0.02	0.40
3III-a	1	341.02	0.1421	0.86	0.85	4.15	3.58	0.38
4III-a	2	339.28	0.0184	0.91	0.90	0.51	0.46	0.30
5III-a	2	343.81	0.0154	0.90	0.88	0.60	0.56	0.33
1III-b	5	241.60	0.0405	0.49	0.49	0.00	0.00	0.81
4III-b	5	276.39	0.7044	0.54	0.54	0.00	0.00	0.76
3III-b	3	321.87	1.1908	0.54	0.53	0.00	0.00	0.78
4III-b	1	363.81	1.6554	0.52	0.51	0.00	0.01	0.79
5III-b	1	403.10	2.1079	0.50	0.50	0.01	0.01	0.80

#	t	λ	f	$\tilde{\chi}_-$	$\tilde{\chi}_+$	$\tilde{\zeta}_{\pm}$	ζ	ϕ_S
1III-c	3	257.53	0.3410	0.66	0.66	2.04	1.30	0.65
2III-c	2	303.80	0.6996	0.67	0.67	3.10	1.98	0.67
3III-c	1	349.45	1.0756	0.66	0.66	4.18	2.41	0.75
4III-c	1	393.40	1.4379	0.66	0.66	5.32	2.87	0.78
5III-c	1	436.05	1.7712	0.66	0.66	6.48	3.51	0.77
1III-d	2	275.52	0.4033	0.67	0.68	2.07	1.35	0.65
2III-d	1	320.74	0.8109	0.68	0.68	3.14	2.01	0.69
3III-d	1	366.95	1.2081	0.67	0.67	4.21	2.51	0.74
4III-d	1	411.59	1.5779	0.66	0.66	5.37	3.29	0.70
5III-d	1	454.89	1.9114	0.67	0.66	6.51	3.93	0.72
1V-NH	1	335.46	0.3938	0.66	0.66	3.13	1.95	0.70
2V-NH	1	431.04	0.4577	0.77	0.77	5.59	4.11	0.60
3V-NH	1	476.22	0.4524	0.83	0.83	7.84	6.20	0.53
4V-NH	1	519.82	0.3941	0.87	0.87	10.00	8.58	0.41
5V-NH	1	548.10	0.3256	0.90	0.91	12.08	10.81	0.34
1V-O	1	334.40	0.3917	0.68	0.68	3.04	1.97	0.68
2V-O	1	423.89	0.5479	0.74	0.74	5.20	3.74	0.60
3V-O	1	493.14	0.6273	0.78	0.79	7.40	5.70	0.53
4V-O	1	545.82	0.6405	0.82	0.83	9.56	7.76	0.47
5V-O	1	583.01	0.6194	0.84	0.85	11.81	9.93	0.42
1V-S	1	344.11	0.3769	0.65	0.65	3.01	1.87	0.71
2V-S	1	443.48	0.5809	0.69	0.70	5.32	3.24	0.73
3V-S	1	514.50	0.7077	0.75	0.75	7.82	5.00	0.70
4V-S	1	565.16	0.7632	0.78	0.79	10.27	7.34	0.62
5V-S	1	598.17	0.7661	0.81	0.81	12.73	9.53	0.58
1V-Se	1	349.77	0.3681	0.63	0.63	2.94	1.78	0.72
2V-Se	1	456.15	0.5976	0.66	0.66	5.16	3.25	0.69
3V-Se	1	533.38	0.7864	0.71	0.71	7.58	5.11	0.65
4V-Se	1	590.26	0.9009	0.74	0.75	10.01	7.29	0.58
5V-Se	1	631.52	0.9591	0.77	0.78	12.43	9.53	0.53
1VI-a	1	321.84	0.0165	0.87	0.85	0.47	0.41	0.39
2VI-a	1	303.40	0.3277	0.69	0.72	0.80	0.53	0.62
3VI-a	1	325.59	1.3178	0.57	0.56	0.03	0.01	0.77
4VI-a	1	341.70	1.6383	0.59	0.58	0.13	0.09	0.73
5VI-a	1	351.16	1.9162	0.60	0.60	0.08	0.04	0.72

#	t	λ	f	$\tilde{\chi}_-$	$\tilde{\chi}_+$	$\tilde{\zeta}_{\pm}$	ζ	ϕ_S
1VI-b	4	285.29	0.0206	0.68	0.68	0.00	0.00	0.67
2VI-b	3	300.88	0.7245	0.58	0.59	0.01	0.01	0.74
3VI-b	1	332.47	1.0304	0.62	0.63	0.03	0.02	0.71
4VI-b	1	351.41	1.2614	0.66	0.66	0.03	0.04	0.68
5VI-b	1	363.41	1.4019	0.69	0.69	0.18	0.07	0.65
1VI-c	1	322.79	0.4135	0.75	0.75	4.00	2.93	0.60
2VI-c	1	403.83	0.4484	0.83	0.84	7.17	5.80	0.49
3VI-c	1	441.44	0.3540	0.89	0.90	10.46	8.48	0.50
4VI-c	1	455.43	0.2380	0.92	0.93	13.99	12.46	0.36
5VI-c	1	458.86	0.1394	0.96	0.96	17.78	16.81	0.23
VII	1	373.57	0.0385	0.48	0.49	2.26	1.06	0.82
VIII	1	344.61	1.4854	0.49	0.49	0.61	0.29	0.77
IX-a	1	456.61	1.3875	0.63	0.63	4.45	2.46	0.75
IX-b	1	532.65	0.6196	0.73	0.73	4.23	3.00	0.60

PBE0 - acetonitrile

#	t	λ	f	$\tilde{\chi}_-$	$\tilde{\chi}_+$	$\tilde{\zeta}_\pm$	ζ	ϕ_S
I-a	1	242.90	0.3237	0.57	0.57	1.27	0.71	0.72
I-b	1	260.78	0.4660	0.58	0.57	0.85	0.48	0.71
1II-a	1	309.96	0.9051	0.56	0.56	0.61	0.33	0.74
2II-a	1	375.46	1.4639	0.56	0.56	0.37	0.19	0.76
3II-a	1	442.38	1.9409	0.57	0.56	0.64	0.34	0.74
4II-a	1	505.19	2.4176	0.58	0.57	1.28	0.69	0.73
5II-a	1	566.15	2.8684	0.58	0.58	2.08	1.14	0.73
1II-b	1	324.81	1.0237	0.55	0.56	0.41	0.22	0.73
2II-b	1	391.80	1.6057	0.57	0.57	0.35	0.18	0.77
3II-b	1	458.93	2.0896	0.57	0.57	0.50	0.27	0.73
4II-b	1	522.47	2.5797	0.58	0.58	0.83	0.46	0.73
5II-b	1	584.63	3.0491	0.58	0.59	1.22	0.67	0.73
1III-a	2	279.49	0.0689	0.84	0.84	0.66	0.56	0.38
2III-a	2	311.16	0.4176	0.71	0.71	0.01	0.01	0.56
3III-a	2	327.69	0.0214	0.87	0.86	0.23	0.21	0.35
4III-a	2	324.82	0.0470	0.86	0.85	0.06	0.05	0.44
5III-a	2	325.77	0.0111	0.68	0.68	0.46	0.32	0.60
1III-b	5	242.14	0.1556	0.45	0.45	0.00	0.00	0.83
2III-b	3	300.55	0.8229	0.57	0.57	0.00	0.00	0.75
3III-b	1	359.43	1.2948	0.56	0.56	0.00	0.00	0.76
4III-b	1	413.36	1.7612	0.55	0.55	0.01	0.01	0.77
5III-b	1	463.42	2.2184	0.54	0.54	0.01	0.01	0.77
1III-c	2	279.37	0.4521	0.62	0.62	1.79	1.07	0.68
2III-c	1	342.82	0.8750	0.64	0.64	2.47	1.50	0.69
3III-c	1	404.88	1.3215	0.65	0.64	3.12	1.91	0.70
4III-c	1	464.99	1.7608	0.65	0.65	3.88	2.37	0.70
5III-c	1	524.20	2.1727	0.65	0.65	4.77	2.93	0.69

#	t	λ	f	$\tilde{\chi}_-$	$\tilde{\chi}_+$	$\tilde{\zeta}_{\pm}$	ζ	ϕ_S
1III-d	2	297.74	0.5020	0.63	0.63	1.67	1.02	0.68
2III-d	1	359.94	1.0115	0.64	0.64	2.49	1.52	0.70
3III-d	1	422.26	1.4849	0.65	0.64	3.00	1.83	0.70
4III-d	1	483.19	1.9448	0.65	0.65	3.60	2.20	0.70
5III-d	1	543.14	2.3748	0.65	0.65	4.39	2.69	0.70
1V-NH	1	367.37	0.5328	0.60	0.60	2.92	1.64	0.75
2V-NH	1	501.22	0.6404	0.72	0.73	5.58	3.88	0.64
3V-NH	1	595.14	0.5776	0.81	0.82	8.21	6.29	0.55
4V-NH	1	632.40	0.4910	0.86	0.87	10.35	8.83	0.42
5V-NH	1	660.38	0.4093	0.89	0.90	12.46	10.64	0.40
1V-O	1	366.27	0.5421	0.62	0.62	2.68	1.57	0.73
2V-O	1	495.80	0.7366	0.72	0.72	5.01	3.44	0.64
3V-O	1	599.09	0.7564	0.79	0.79	7.55	5.83	0.54
4V-O	1	664.24	0.6906	0.84	0.84	9.96	8.28	0.45
5V-O	1	696.47	0.6121	0.87	0.87	12.36	10.73	0.38
1V-S	1	376.21	0.5277	0.61	0.61	2.71	1.58	0.74
2V-S	1	515.79	0.8093	0.67	0.68	5.09	3.29	0.68
3V-S	1	624.27	0.9160	0.74	0.75	7.88	5.40	0.65
4V-S	1	688.36	0.8860	0.79	0.81	10.60	7.93	0.58
5V-S	1	713.98	0.8169	0.83	0.84	13.31	10.79	0.49
1V-Se	1	380.98	0.5162	0.59	0.59	2.60	1.47	0.75
2V-Se	1	527.16	0.8396	0.63	0.64	4.75	2.89	0.70
3V-Se	1	645.22	1.0374	0.70	0.70	7.55	5.12	0.64
4V-Se	1	728.27	1.1002	0.75	0.76	10.27	7.60	0.57
5V-Se	1	772.66	1.0995	0.79	0.79	12.90	10.08	0.51
1VI-a	1	319.78	0.0655	0.64	0.64	0.00	0.00	0.68
2VI-a	2	310.81	1.0629	0.53	0.58	0.72	0.37	0.80
3VI-a	1	346.69	1.5133	0.60	0.58	0.04	0.04	0.74
4VI-a	1	366.66	1.8072	0.61	0.62	0.13	0.04	0.72
5VI-a	1	376.43	2.0380	0.63	0.63	0.31	0.19	0.69

#	t	λ	f	$\tilde{\chi}_-$	$\tilde{\chi}_+$	$\tilde{\zeta}_{\pm}$	ζ	ϕ_S
1VI-b	3	304.24	0.0291	0.74	0.74	0.00	0.00	0.61
2VI-b	1	327.38	0.8835	0.62	0.63	0.01	0.01	0.72
3VI-b	1	367.88	1.1767	0.68	0.68	0.03	0.02	0.65
4VI-b	1	391.84	1.3338	0.72	0.72	0.05	0.04	0.61
5VI-b	1	405.63	1.4078	0.75	0.74	0.13	0.06	0.58
1VI-c	1	364.81	0.5528	0.74	0.74	3.93	2.84	0.62
2VI-c	1	481.69	0.5725	0.84	0.85	7.28	5.64	0.57
3VI-c	1	519.15	0.3910	0.91	0.91	10.76	9.44	0.40
4VI-c	1	519.26	0.2424	0.93	0.94	14.40	13.50	0.24
5VI-c	1	509.80	0.1363	0.96	0.96	18.28	17.51	0.17
VII	1	388.52	0.0853	0.53	0.53	2.37	1.22	0.77
VIII	1	366.92	1.7194	0.52	0.53	0.62	0.33	0.75
IX-a	1	544.52	1.4647	0.65	0.65	4.49	2.61	0.73
IX-b	1	633.57	0.4708	0.78	0.78	5.57	4.14	0.56

B3LYP - vacuum

#	t	λ	f	$\tilde{\chi}_-$	$\tilde{\chi}_+$	$\tilde{\zeta}_\pm$	ζ	ϕ_S
I-a	1	244.83	0.2619	0.57	0.57	1.35	0.75	0.74
I-b	1	259.01	0.4031	0.59	0.58	0.93	0.53	0.72
1II-a	1	297.88	0.7895	0.54	0.54	0.06	0.03	0.76
2II-a	1	343.00	1.2516	0.55	0.55	1.71	0.83	0.79
3II-a	1	399.79	1.6942	0.57	0.57	3.09	1.56	0.76
4II-a	1	447.89	2.0370	0.60	0.60	4.68	2.37	0.78
5II-a	1	494.94	2.3142	0.64	0.64	6.21	3.25	0.78
1II-b	1	314.21	0.9047	0.56	0.56	0.25	0.12	0.77
2II-b	1	360.79	1.3871	0.57	0.57	1.93	0.95	0.79
3II-b	1	418.08	1.8339	0.59	0.59	3.13	1.65	0.75
4II-b	1	466.76	2.1821	0.61	0.62	4.68	2.53	0.75
5II-b	1	514.43	2.4605	0.63	0.65	6.04	3.48	0.72
1III-a	2	311.99	0.0297	0.88	0.88	0.70	0.62	0.31
2III-a	2	345.59	0.1088	0.86	0.87	0.01	0.02	0.37
3III-a	1	364.70	0.0183	0.90	0.88	0.58	0.51	0.30
4III-a	2	365.23	0.0163	0.91	0.90	0.44	0.41	0.31
5III-a	2	370.50	0.0140	0.90	0.90	0.54	0.51	0.33
1III-b	5	251.55	0.0304	0.51	0.50	0.00	0.00	0.80
2III-b	5	284.09	0.6733	0.55	0.55	0.00	0.00	0.75
3III-b	3	330.85	1.1522	0.55	0.55	0.00	0.00	0.77
4III-b	1	374.15	1.6050	0.54	0.53	0.01	0.01	0.78
5III-b	1	414.90	2.0458	0.52	0.51	0.01	0.01	0.79
1III-c	3	263.71	0.3260	0.67	0.66	2.08	1.34	0.65
2III-c	2	311.41	0.6656	0.69	0.69	3.21	2.10	0.66
3III-c	1	358.69	1.0162	0.69	0.69	4.37	2.58	0.74
4III-c	1	404.44	1.3486	0.69	0.69	5.60	3.06	0.78
5III-c	1	449.18	1.6475	0.69	0.69	6.86	3.83	0.76

#	t	λ	f	$\tilde{\chi}_-$	$\tilde{\chi}_+$	$\tilde{\zeta}_{\pm}$	ζ	ϕ_S
1III-d	2	282.14	0.3905	0.68	0.68	2.14	1.41	0.64
2III-d	1	328.68	0.7747	0.70	0.70	3.25	2.11	0.69
3III-d	1	376.42	1.1469	0.69	0.69	4.42	2.67	0.73
4III-d	1	422.82	1.4876	0.69	0.69	5.66	3.55	0.69
5III-d	1	468.22	1.7877	0.70	0.69	6.90	4.28	0.71
1V-NH	1	344.31	0.3812	0.67	0.67	3.21	2.02	0.69
2V-NH	1	452.38	0.4217	0.79	0.79	5.76	4.29	0.59
3V-NH	1	512.28	0.3905	0.85	0.85	8.13	6.58	0.51
4V-NH	1	571.66	0.3213	0.89	0.89	10.37	9.11	0.38
5V-NH	1	613.69	0.2506	0.92	0.92	12.53	11.49	0.30
1V-O	1	343.18	0.3796	0.69	0.69	3.12	2.01	0.69
2V-O	1	441.88	0.5082	0.76	0.77	5.38	3.96	0.59
3V-O	1	523.71	0.5508	0.81	0.82	7.69	6.13	0.50
4V-O	1	590.90	0.5291	0.85	0.86	9.96	8.37	0.43
5V-O	1	642.41	0.4786	0.88	0.88	12.33	10.78	0.37
1V-S	1	353.29	0.3660	0.66	0.66	3.10	1.95	0.71
2V-S	1	461.89	0.5462	0.71	0.72	5.56	3.43	0.72
3V-S	1	546.17	0.6300	0.78	0.78	8.21	5.40	0.69
4V-S	1	611.71	0.6357	0.82	0.83	10.79	8.01	0.59
5V-S	1	658.98	0.5912	0.85	0.85	13.40	10.43	0.54
1V-Se	1	358.75	0.3572	0.64	0.64	3.04	1.86	0.72
2V-Se	1	473.37	0.5660	0.68	0.68	5.41	3.50	0.67
3V-Se	1	562.34	0.7120	0.74	0.74	8.00	5.60	0.63
4V-Se	1	633.28	0.7691	0.78	0.79	10.62	8.10	0.54
5V-Se	1	688.99	0.7659	0.82	0.82	13.22	10.72	0.47
1VI-a	2	320.47	0.0572	0.88	0.87	0.00	0.01	0.33
2VI-a	1	321.02	0.1191	0.80	0.79	0.53	0.41	0.51
3VI-a	1	336.31	1.2267	0.58	0.56	0.01	0.02	0.76
4VI-a	1	354.60	1.4991	0.60	0.59	0.07	0.05	0.72
5VI-a	1	365.93	1.7027	0.62	0.62	0.09	0.06	0.70

#	t	λ	f	$\tilde{\chi}_-$	$\tilde{\chi}_+$	$\tilde{\zeta}_{\pm}$	ζ	ϕ_S
1VI-b	3	297.05	0.0191	0.71	0.71	0.00	0.00	0.65
2VI-b	3	313.12	0.6461	0.60	0.60	0.01	0.00	0.73
3VI-b	1	349.84	0.9377	0.66	0.66	0.03	0.02	0.67
4VI-b	1	373.32	1.0747	0.70	0.71	0.05	0.02	0.63
5VI-b	1	389.32	1.1124	0.74	0.74	0.21	0.11	0.59
1VI-c	1	335.50	0.3890	0.77	0.77	4.11	3.06	0.59
2VI-c	1	432.19	0.3959	0.86	0.86	7.37	6.13	0.46
3VI-c	1	485.48	0.2861	0.92	0.92	10.74	9.08	0.46
4VI-c	1	509.76	0.1738	0.94	0.95	14.30	13.19	0.30
5VI-c	1	518.95	0.0923	0.97	0.97	18.12	17.39	0.19
VII	1	394.78	0.0266	0.47	0.48	2.21	0.99	0.83
VIII	1	356.56	1.3970	0.49	0.49	0.62	0.30	0.77
IX-a	1	473.35	1.2766	0.66	0.66	5.02	2.95	0.71
IX-b	1	566.76	0.4886	0.75	0.75	4.43	3.22	0.58

B3LYP - acetonitrile

#	t	λ	f	$\tilde{\chi}_-$	$\tilde{\chi}_+$	$\tilde{\zeta}_\pm$	ζ	ϕ_S
I-a	1	247.23	0.3113	0.58	0.57	1.34	0.75	0.72
I-b	1	265.44	0.4501	0.58	0.58	0.92	0.52	0.70
1II-a	1	314.12	0.8846	0.56	0.56	0.67	0.36	0.74
2II-a	1	379.97	1.4360	0.57	0.57	0.34	0.17	0.77
3II-a	1	446.57	1.9127	0.57	0.57	0.61	0.33	0.73
4II-a	1	509.53	2.3845	0.58	0.58	1.29	0.70	0.73
5II-a	1	570.82	2.8283	0.59	0.58	2.15	1.18	0.73
1II-b	1	329.04	1.0019	0.56	0.56	0.45	0.24	0.73
2II-b	1	396.41	1.5755	0.57	0.57	0.33	0.17	0.77
3II-b	1	463.15	2.0590	0.58	0.57	0.48	0.26	0.73
4II-b	1	526.64	2.5447	0.59	0.58	0.81	0.44	0.73
5II-b	1	588.80	3.0081	0.59	0.59	1.22	0.67	0.73
1III-a	2	296.38	0.0580	0.86	0.85	0.63	0.55	0.36
2III-a	2	329.28	0.2806	0.78	0.78	0.01	0.02	0.49
3III-a	2	348.34	0.0208	0.87	0.86	0.23	0.21	0.35
4III-a	2	344.94	0.0973	0.84	0.83	0.16	0.13	0.46
5III-a	2	346.96	0.0145	0.81	0.81	0.38	0.32	0.47
1III-b	5	250.71	0.1167	0.43	0.43	0.00	0.00	0.84
2III-b	3	309.83	0.7985	0.58	0.58	0.00	0.00	0.74
3III-b	1	371.06	1.2581	0.58	0.58	0.00	0.00	0.75
4III-b	1	427.26	1.7129	0.57	0.57	0.01	0.01	0.76
5III-b	1	479.64	2.1587	0.56	0.56	0.01	0.01	0.76
1III-c	2	285.17	0.4385	0.63	0.63	1.83	1.10	0.68
2III-c	1	349.57	0.8489	0.65	0.65	2.57	1.57	0.69
3III-c	1	412.60	1.2813	0.66	0.66	3.29	2.03	0.69
4III-c	1	473.85	1.7053	0.66	0.66	4.12	2.55	0.69
5III-c	1	534.59	2.1000	0.67	0.67	5.09	3.18	0.69

#	t	λ	f	$\tilde{\chi}_-$	$\tilde{\chi}_+$	$\tilde{\zeta}_{\pm}$	ζ	ϕ_S
1III-d	2	303.95	0.5264	0.63	0.63	1.98	1.21	0.68
2III-d	1	366.69	0.9835	0.65	0.65	2.59	1.59	0.70
3III-d	1	429.67	1.4438	0.66	0.65	3.16	1.95	0.70
4III-d	1	491.38	1.8910	0.66	0.66	3.83	2.37	0.70
5III-d	1	552.46	2.3063	0.67	0.66	4.69	2.92	0.70
1V-NH	1	375.37	0.5190	0.60	0.60	2.99	1.67	0.75
2V-NH	1	523.73	0.6075	0.73	0.74	5.75	4.01	0.64
3V-NH	1	645.82	0.5263	0.83	0.83	8.45	6.51	0.53
4V-NH	1	708.76	0.4239	0.88	0.88	10.70	9.27	0.41
5V-NH	1	757.68	0.3347	0.91	0.91	12.94	11.25	0.38
1V-O	1	373.72	0.5303	0.63	0.63	2.74	1.58	0.75
2V-O	1	513.83	0.7039	0.73	0.73	5.19	3.59	0.64
3V-O	1	639.51	0.6948	0.81	0.81	7.83	6.15	0.53
4V-O	1	733.64	0.6012	0.86	0.87	10.34	8.80	0.43
5V-O	1	790.95	0.4984	0.89	0.90	12.84	11.46	0.35
1V-S	1	384.52	0.5154	0.61	0.62	2.79	1.62	0.74
2V-S	1	534.12	0.7792	0.69	0.69	5.28	3.44	0.67
3V-S	1	664.59	0.8488	0.77	0.77	8.22	5.70	0.64
4V-S	1	758.72	0.7704	0.83	0.83	11.09	8.52	0.57
5V-S	1	809.81	0.6543	0.87	0.87	13.95	11.76	0.45
1V-Se	1	389.26	0.5020	0.60	0.60	2.69	1.53	0.75
2V-Se	1	543.63	0.8097	0.65	0.65	4.94	3.04	0.70
3V-Se	1	679.86	0.9714	0.72	0.73	7.91	5.49	0.63
4V-Se	1	790.21	0.9795	0.78	0.79	10.83	8.30	0.54
5V-Se	1	862.73	0.9110	0.83	0.83	13.63	11.16	0.46
1VI-a	1	326.55	0.0636	0.64	0.64	0.00	0.00	0.67
2VI-a	2	320.40	0.8643	0.55	0.61	0.96	0.51	0.77
3VI-a	1	358.01	1.4229	0.60	0.59	0.03	0.02	0.73
4VI-a	1	380.92	1.6623	0.63	0.63	0.16	0.06	0.70
5VI-a	1	393.11	1.8178	0.65	0.66	0.32	0.19	0.67

#	t	λ	f	$\tilde{\chi}_-$	$\tilde{\chi}_+$	$\tilde{\zeta}_{\pm}$	ζ	ϕ_S
1VI-b	3	319.22	0.0264	0.76	0.76	0.00	0.00	0.58
2VI-b	1	343.48	0.8445	0.65	0.65	0.02	0.02	0.70
3VI-b	1	392.11	1.0630	0.71	0.71	0.03	0.01	0.62
4VI-b	1	423.41	1.1365	0.76	0.76	0.07	0.04	0.57
5VI-b	1	443.21	1.1190	0.80	0.79	0.19	0.11	0.52
1VI-c	1	379.03	0.5277	0.75	0.75	4.04	2.94	0.62
2VI-c	1	521.72	0.5231	0.86	0.86	7.46	5.91	0.55
3VI-c	1	586.24	0.3293	0.93	0.93	11.00	9.82	0.38
4VI-c	1	597.80	0.1846	0.95	0.96	14.66	13.98	0.21
5VI-c	1	591.58	0.0940	0.98	0.98	18.56	18.03	0.14
VII	1	409.55	0.0597	0.52	0.52	2.33	1.18	0.78
VIII	1	378.98	1.6417	0.52	0.53	0.65	0.34	0.74
IX-a	1	568.98	1.3405	0.67	0.68	5.18	3.17	0.69
IX-b	1	677.62	0.3624	0.80	0.80	5.79	4.44	0.54

CAM-B3LYP - vacuum

#	t	λ	f	$\tilde{\chi}_-$	$\tilde{\chi}_+$	$\tilde{\zeta}_{\pm}$	ζ	ϕ_S
I-a	1	237.09	0.3027	0.55	0.55	0.95	0.51	0.76
I-b	1	249.40	0.4520	0.57	0.56	0.61	0.34	0.73
1II-a	1	291.74	0.8471	0.53	0.53	0.29	0.15	0.76
2II-a	1	330.32	1.3483	0.52	0.52	1.56	0.74	0.80
3II-a	1	386.20	1.7813	0.53	0.53	2.43	1.20	0.78
4II-a	1	425.36	2.2038	0.53	0.53	3.39	1.61	0.80
5II-a	1	460.45	2.6100	0.53	0.53	4.25	2.04	0.81
1II-b	1	307.33	0.9538	0.54	0.55	0.44	0.22	0.77
2II-b	1	347.32	1.4733	0.54	0.54	1.65	0.81	0.79
3II-b	1	403.75	1.9192	0.54	0.55	2.44	1.26	0.77
4II-b	1	443.58	2.3473	0.54	0.55	3.37	1.74	0.78
5II-b	1	479.13	2.7538	0.54	0.55	4.10	2.13	0.77
1III-a	1	297.48	0.0373	0.86	0.85	0.17	0.15	0.35
2III-a	2	295.63	0.1168	0.83	0.83	0.01	0.03	0.41
3III-a	1	314.62	0.9352	0.57	0.55	1.15	0.64	0.72
4III-a	1	342.57	1.8722	0.47	0.46	0.62	0.26	0.85
5III-a	1	372.81	2.4903	0.44	0.45	0.25	0.11	0.85
1III-b	5	223.42	0.1377	0.45	0.45	0.00	0.00	0.84
2III-b	5	264.35	0.7562	0.51	0.51	0.00	0.00	0.78
3III-b	3	305.03	1.2512	0.49	0.49	0.00	0.00	0.80
4III-b	1	341.44	1.7393	0.47	0.46	0.00	0.01	0.82
5III-b	1	374.53	2.2176	0.45	0.45	0.00	0.01	0.82
1III-c	3	254.57	0.3542	0.65	0.65	1.92	1.21	0.66
2III-c	2	295.17	0.7504	0.63	0.63	2.69	1.63	0.71
3III-c	1	334.19	1.1902	0.59	0.59	3.39	1.79	0.78
4III-c	1	370.53	1.6348	0.57	0.57	4.07	1.99	0.81
5III-c	1	404.17	2.0679	0.55	0.55	4.72	2.21	0.82

#	t	λ	f	$\tilde{\chi}_-$	$\tilde{\chi}_+$	$\tilde{\zeta}_{\pm}$	ζ	ϕ_S
1III-d	2	270.73	0.4147	0.66	0.66	1.91	1.22	0.66
2III-d	1	310.67	0.8612	0.64	0.64	2.67	1.62	0.71
3III-d	1	350.53	1.3199	0.61	0.60	3.33	1.86	0.76
4III-d	1	387.47	1.7711	0.58	0.58	4.04	2.22	0.76
5III-d	1	421.44	2.2045	0.56	0.56	4.69	2.50	0.77
1V-NH	1	325.50	0.4162	0.64	0.64	2.75	1.68	0.70
2V-NH	1	380.49	0.6003	0.68	0.68	4.48	2.92	0.68
3V-NH	1	386.97	0.8070	0.69	0.69	5.54	3.55	0.70
4V-NH	1	394.36	1.0031	0.68	0.69	6.30	4.18	0.66
5V-NH	1	396.47	1.2131	0.67	0.68	6.73	4.40	0.67
1V-O	1	322.58	0.4097	0.65	0.65	2.69	1.69	0.70
2V-O	1	381.30	0.6702	0.65	0.65	4.12	2.61	0.69
3V-O	1	412.29	0.9616	0.62	0.62	5.32	3.25	0.70
4V-O	1	428.54	1.2890	0.59	0.59	6.05	3.53	0.72
5V-O	1	437.28	1.6671	0.55	0.56	6.22	3.43	0.75
1V-S	1	332.91	0.3914	0.62	0.62	2.53	1.52	0.72
2V-S	1	403.49	0.6650	0.60	0.60	3.98	2.10	0.80
3V-S	1	435.85	0.9791	0.58	0.58	5.20	2.52	0.82
4V-S	1	451.29	1.3369	0.55	0.55	5.81	2.82	0.81
5V-S	1	458.22	1.7368	0.53	0.52	5.81	2.75	0.82
1V-Se	1	339.88	0.3810	0.61	0.61	2.42	1.43	0.73
2V-Se	1	420.71	0.6614	0.57	0.57	3.78	2.12	0.75
3V-Se	1	462.19	1.0010	0.55	0.56	4.95	2.65	0.76
4V-Se	1	483.29	1.3753	0.53	0.53	5.57	2.90	0.77
5V-Se	1	495.14	1.7902	0.51	0.51	5.77	2.90	0.78
1VI-a	1	298.83	0.0215	0.85	0.84	0.35	0.28	0.50
2VI-a	2	283.24	0.4619	0.64	0.63	0.03	0.04	0.68
3VI-a	1	296.34	1.4819	0.50	0.49	0.02	0.02	0.83
4VI-a	1	303.95	2.0402	0.49	0.48	0.12	0.06	0.82
5VI-a	1	307.90	2.6139	0.47	0.47	0.09	0.03	0.83

#	t	λ	f	$\tilde{\chi}_-$	$\tilde{\chi}_+$	$\tilde{\zeta}_\pm$	ζ	ϕ_S
1VI-b	5	267.78	0.0262	0.60	0.60	0.00	0.00	0.74
2VI-b	3	277.79	0.8187	0.53	0.54	0.01	0.01	0.78
3VI-b	3	295.43	1.2815	0.52	0.52	0.04	0.01	0.79
4VI-b	3	303.40	1.2810	0.55	0.55	0.03	0.02	0.75
5VI-b	1	309.29	2.0196	0.51	0.52	0.13	0.03	0.79
1VI-c	5	240.86	0.0299	0.87	0.86	1.89	1.64	0.32
2VI-c	3	275.54	0.0276	0.49	0.50	1.50	0.70	0.80
3VI-c	3	275.93	0.0252	0.52	0.52	1.07	0.54	0.80
4VI-c	3	279.66	0.0526	0.56	0.56	5.48	2.77	0.81
5VI-c	1	316.93	2.0864	0.52	0.52	7.90	3.88	0.79
VII	1	334.50	1.4846	0.44	0.45	1.50	0.62	0.84
VIII	1	314.86	1.7377	0.49	0.49	0.55	0.27	0.79
IX-a	1	413.02	1.7223	0.53	0.53	1.82	0.79	0.84
IX-b	1	463.13	1.0028	0.64	0.65	2.76	1.74	0.69

CAM-B3LYP - acetonitrile

#	t	λ	f	$\tilde{\chi}_-$	$\tilde{\chi}_+$	$\tilde{\zeta}_{\pm}$	ζ	ϕ_S
I-a	1	239.97	0.3498	0.56	0.56	1.02	0.56	0.73
I-b	1	256.32	0.4905	0.57	0.57	0.70	0.39	0.71
1II-a	1	309.91	0.9342	0.55	0.55	0.41	0.22	0.74
2II-a	1	376.60	1.4943	0.56	0.56	0.50	0.26	0.76
3II-a	1	447.27	1.9533	0.56	0.56	0.71	0.39	0.74
4II-a	1	511.77	2.4276	0.57	0.56	1.17	0.65	0.74
5II-a	1	572.84	2.8826	0.57	0.56	1.74	0.97	0.74
1II-b	1	323.43	1.0431	0.55	0.55	0.36	0.20	0.74
2II-b	1	392.40	1.6254	0.56	0.56	0.42	0.21	0.78
3II-b	1	464.09	2.0940	0.57	0.56	0.56	0.31	0.74
4II-b	1	531.23	2.5788	0.57	0.57	0.79	0.44	0.74
5II-b	1	596.78	3.0471	0.57	0.57	1.06	0.60	0.74
1III-a	2	259.94	0.0010	0.88	0.89	0.05	0.05	0.30
2III-a	2	291.85	0.6272	0.61	0.61	0.01	0.01	0.67
3III-a	2	310.15	0.0201	0.87	0.87	0.05	0.06	0.38
4III-a	2	308.52	0.0304	0.87	0.86	0.12	0.11	0.42
5III-a	2	307.57	0.0128	0.87	0.87	0.10	0.12	0.37
1III-b	5	231.13	0.3030	0.53	0.53	0.00	0.00	0.72
2III-b	3	287.80	0.8538	0.54	0.54	0.00	0.00	0.77
3III-b	1	340.29	1.3436	0.53	0.53	0.00	0.00	0.78
4III-b	1	386.88	1.8326	0.51	0.51	0.01	0.00	0.79
5III-b	1	428.53	2.3153	0.50	0.49	0.00	0.01	0.80
1III-c	2	281.51	0.4574	0.62	0.62	1.69	1.02	0.68
2III-c	1	343.53	0.8949	0.62	0.62	2.15	1.30	0.70
3III-c	1	403.44	1.3663	0.61	0.61	2.55	1.52	0.71
4III-c	1	459.90	1.8353	0.61	0.60	3.00	1.77	0.72
5III-c	1	512.51	2.2854	0.60	0.60	3.56	2.08	0.73

#	t	λ	f	$\tilde{\chi}_-$	$\tilde{\chi}_+$	$\tilde{\zeta}_{\pm}$	ζ	ϕ_S
1III-d	1	298.32	0.5496	0.62	0.62	1.78	1.07	0.68
2III-d	1	360.30	1.0245	0.62	0.62	2.09	1.25	0.71
3III-d	1	422.06	1.5177	0.62	0.61	2.38	1.42	0.72
4III-d	1	481.35	2.0012	0.61	0.61	2.73	1.62	0.72
5III-d	1	537.19	2.4603	0.60	0.60	3.23	1.91	0.73
1V-NH	1	364.12	0.5627	0.57	0.57	2.48	1.35	0.75
2V-NH	1	450.37	0.7733	0.66	0.66	4.49	2.89	0.69
3V-NH	1	466.20	0.9196	0.70	0.71	6.03	4.04	0.66
4V-NH	1	458.18	1.0781	0.71	0.71	6.73	4.58	0.65
5V-NH	1	456.29	1.2429	0.70	0.70	7.10	4.84	0.65
1V-O	1	363.47	0.5589	0.60	0.60	2.32	1.34	0.73
2V-O	1	456.63	0.8290	0.66	0.66	4.02	2.59	0.69
3V-O	1	486.87	1.0464	0.66	0.67	5.67	3.73	0.67
4V-O	1	486.23	1.3054	0.64	0.64	6.73	4.31	0.68
5V-O	1	480.72	1.6499	0.60	0.61	6.99	4.23	0.71
1V-S	1	372.52	0.5465	0.59	0.59	2.24	1.29	0.74
2V-S	1	480.80	0.8778	0.62	0.62	3.91	2.35	0.72
3V-S	1	520.10	1.1635	0.62	0.62	5.56	3.16	0.75
4V-S	1	518.73	1.4858	0.58	0.59	6.44	3.40	0.78
5V-S	1	510.11	1.8984	0.55	0.55	6.51	3.32	0.79
1V-Se	1	378.59	0.5373	0.58	0.58	2.11	1.19	0.75
2V-Se	1	501.34	0.8954	0.59	0.59	3.56	2.05	0.74
3V-Se	1	558.24	1.2281	0.59	0.59	5.19	3.02	0.73
4V-Se	1	572.34	1.5801	0.56	0.57	6.20	3.48	0.74
5V-Se	1	570.72	2.0025	0.53	0.53	6.33	3.33	0.77
1VI-a	1	304.19	0.0785	0.59	0.59	0.00	0.00	0.72
2VI-a	2	291.51	1.0626	0.52	0.51	0.12	0.06	0.82
3VI-a	1	312.43	1.7112	0.52	0.51	0.03	0.01	0.80
4VI-a	1	321.11	2.2689	0.51	0.51	0.16	0.05	0.82
5VI-a	1	323.90	2.8460	0.49	0.49	0.28	0.15	0.82

#	t	λ	f	$\tilde{\chi}_-$	$\tilde{\chi}_+$	$\tilde{\zeta}_\pm$	ζ	ϕ_S
1VI-b	3	283.33	0.0386	0.67	0.66	0.00	0.00	0.68
2VI-b	3	299.35	0.9129	0.57	0.57	0.05	0.02	0.75
3VI-b	1	321.66	1.4763	0.57	0.58	0.02	0.02	0.74
4VI-b	1	330.15	1.9706	0.56	0.57	0.04	0.03	0.76
5VI-b	1	333.21	2.4773	0.55	0.55	0.09	0.03	0.77
1VI-c	1	340.31	0.6089	0.70	0.70	3.37	2.31	0.65
2VI-c	1	380.42	0.8272	0.72	0.72	6.05	4.00	0.67
3VI-c	1	361.15	1.0364	0.70	0.69	8.39	5.67	0.63
4VI-c	1	344.51	1.4957	0.62	0.62	9.38	5.71	0.69
5VI-c	1	335.46	2.1689	0.55	0.56	8.22	4.36	0.76
VII	1	357.96	1.6559	0.47	0.47	1.49	0.68	0.81
VIII	1	337.70	1.9293	0.52	0.52	0.57	0.29	0.77
IX-a	1	490.79	1.8233	0.56	0.56	1.32	0.62	0.83
IX-b	1	534.86	0.9112	0.65	0.65	3.58	2.25	0.68

The ϕ_S and barycentre-related indices derived from Detachment/Attachment and NTO's density matrices

The thirty-six molecules of the IV set (*Figure 4*) were recently investigated in ref [13] with the barycentre approach. For the sake of consistency, nomenclature from [13] will be used in the following table. No confusion must be made with respect to the nomenclature previously used throughout this article: as recalled in the introduction, the core of each molecule in the following table is the thieno[3,4-b]pyrazine (molecule IV in the *Figure 4*), but its derivatives investigated in the present survey were labelled differently in [13].

#	t	λ	f	$\tilde{\chi}$	$\tilde{\chi}^{\text{NTO}}$	$\tilde{\zeta}_{\pm}$	$\tilde{\zeta}_{\pm}^{\text{NTO}}$	ζ	ζ^{NTO}
II-a	1	341.26	0.0506	0.64	0.64	3.66	3.65	2.29	2.31
II-a	2	337.59	0.0032	0.70	0.70	0.91	0.92	0.63	0.63
II-a	3	276.86	0.3140	0.49	0.49	2.49	2.48	1.18	1.19
II-a	4	225.34	0.0000	0.72	0.71	0.47	0.48	0.33	0.33
II-a	5	210.82	0.0651	0.48	0.47	0.12	0.12	0.06	0.05
II-a	6	205.75	0.0000	0.83	0.83	0.28	0.28	0.24	0.23
II-c	1	348.98	0.0239	0.64	0.64	3.65	3.65	2.28	2.30
II-c	2	311.82	0.0031	0.69	0.69	0.97	0.98	0.67	0.67
II-c	3	295.30	0.4517	0.54	0.54	0.30	0.30	0.16	0.16
II-c	4	255.11	0.0000	0.82	0.82	4.86	4.85	3.94	3.94
II-c	5	216.30	0.0285	0.73	0.73	5.38	5.38	3.93	3.94
II-c	6	214.67	0.0000	0.70	0.70	5.37	5.37	3.73	3.73
II-d	1	324.81	0.0396	0.60	0.60	3.39	3.38	2.01	2.03
II-d	2	323.04	0.0055	0.66	0.66	0.46	0.46	0.30	0.30
II-d	3	278.33	0.4444	0.51	0.51	1.68	1.68	0.83	0.84
II-d	4	226.30	0.0003	0.73	0.73	0.46	0.46	0.30	0.29
II-d	5	225.68	0.0136	0.93	0.93	5.66	5.66	5.26	5.26
II-d	6	214.41	0.0835	0.82	0.82	5.49	5.49	4.43	4.44
II-e	1	326.66	0.0015	0.71	0.71	0.87	0.90	0.61	0.63
II-e	2	317.96	0.0459	0.61	0.60	3.66	3.67	2.16	2.19
II-e	3	275.95	0.4479	0.50	0.50	1.90	1.92	0.93	0.96
II-e	4	225.59	0.0000	0.73	0.73	0.40	0.41	0.28	0.29
II-e	5	211.52	0.0000	0.85	0.85	0.13	0.13	0.16	0.16
II-e	6	211.23	0.0538	0.50	0.50	0.49	0.47	0.26	0.26

#	t	λ	f	$\tilde{\chi}$	$\tilde{\chi}^{\text{NTO}}$	$\tilde{\zeta}_{\pm}$	$\tilde{\zeta}_{\pm}^{\text{NTO}}$	ζ	ζ^{NTO}
II-f	1	330.79	0.0368	0.64	0.63	3.71	3.71	2.30	2.32
II-f	2	320.15	0.0017	0.70	0.70	0.81	0.81	0.57	0.57
II-f	3	278.69	0.4014	0.50	0.50	2.02	2.02	0.98	0.99
II-f	4	238.01	0.0001	0.76	0.76	2.19	2.18	1.59	1.60
II-f	5	210.69	0.0156	0.90	0.90	5.10	5.11	4.62	4.62
II-f	6	210.19	0.0059	0.84	0.84	4.92	4.91	4.10	4.11
II-g	1	371.29	0.0251	0.65	0.65	4.69	4.68	2.99	3.02
II-g	2	315.41	0.0015	0.71	0.70	0.80	0.80	0.56	0.57
II-g	3	308.05	0.4891	0.49	0.49	2.55	2.54	1.21	1.22
II-g	4	223.00	0.0000	0.73	0.73	1.40	1.39	0.96	0.97
II-g	5	216.55	0.4703	0.49	0.49	1.26	1.25	0.61	0.61
II-g	6	209.26	0.1541	0.44	0.44	3.02	3.02	1.31	1.32
II-i	1	400.06	0.0164	0.66	0.66	3.75	3.74	2.40	2.42
II-i	2	335.12	0.0020	0.69	0.69	0.45	0.47	0.31	0.32
II-i	3	305.43	0.2282	0.39	0.39	2.53	2.52	0.97	0.98
II-i	4	250.54	0.0000	0.73	0.73	1.17	1.17	0.83	0.83
II-i	5	243.51	1.2265	0.53	0.53	6.79	6.81	3.48	3.54
II-i	6	224.55	0.1778	0.50	0.50	5.04	5.04	2.49	2.50
III	1	366.17	0.0104	0.58	0.58	0.51	0.50	0.29	0.28
III	2	333.77	0.0022	0.70	0.70	0.17	0.15	0.15	0.13
III	3	322.10	0.0434	0.36	0.36	4.56	4.57	1.63	1.64
III	4	306.43	1.3639	0.46	0.47	0.78	0.75	0.35	0.34
III	5	297.84	0.0003	0.44	0.44	0.74	0.74	0.32	0.32
III	6	286.83	0.0178	0.41	0.41	1.56	1.57	0.64	0.65
IV	1	401.44	0.0254	0.57	0.57	2.10	2.09	1.15	1.16
IV	2	360.74	0.0015	0.69	0.69	0.02	0.02	0.08	0.09
IV	3	342.48	0.6503	0.50	0.50	2.01	2.02	1.00	1.02
IV	4	323.19	0.0253	0.63	0.63	6.28	6.29	3.95	3.96
IV	5	271.52	0.0012	0.35	0.35	1.95	1.96	0.69	0.69
IV	6	265.11	0.2807	0.29	0.29	1.22	1.23	0.35	0.35

#	t	λ	f	$\tilde{\chi}$	$\tilde{\chi}^{\text{NTO}}$	$\tilde{\zeta}_{\pm}$	$\tilde{\zeta}_{\pm}^{\text{NTO}}$	ζ	ζ^{NTO}
V	1	402.34	0.0213	0.58	0.58	3.20	3.18	1.79	1.80
V	2	356.82	0.0017	0.70	0.70	0.04	0.04	0.02	0.02
V	3	329.79	0.6321	0.48	0.48	0.28	0.28	0.14	0.14
V	4	295.15	0.0007	0.60	0.60	6.25	6.25	3.76	3.77
V	5	274.64	0.2024	0.54	0.54	5.20	5.20	2.77	2.78
V	6	274.40	0.0000	0.83	0.83	5.79	5.80	4.74	4.74
VI-a	1	545.07	0.3926	0.56	0.56	3.51	3.50	1.92	1.93
VI-a	2	351.45	0.0020	0.70	0.70	1.58	1.58	1.09	1.09
VI-a	3	316.26	0.4882	0.54	0.54	3.30	3.31	1.76	1.76
VI-a	4	300.54	0.0051	0.40	0.40	4.46	4.49	1.76	1.79
VI-a	5	299.09	0.1514	0.62	0.62	1.35	1.33	0.82	0.82
VI-a	6	278.43	0.0210	0.44	0.44	3.72	3.72	1.61	1.62
VI-b	1	505.71	0.4387	0.53	0.53	3.28	3.29	1.68	1.70
VI-b	2	338.25	0.0016	0.71	0.71	1.57	1.58	1.11	1.12
VI-b	3	307.89	0.4059	0.57	0.57	3.83	3.83	2.14	2.15
VI-b	4	302.13	0.1556	0.43	0.43	0.13	0.13	0.05	0.06
VI-b	5	292.84	0.1930	0.46	0.46	3.57	3.60	1.61	1.63
VI-b	6	273.09	0.0734	0.36	0.36	4.39	4.40	1.52	1.53
VI-c	1	544.58	0.3109	0.56	0.56	3.95	3.93	1.66	1.69
VI-c	2	347.00	0.0058	0.70	0.70	1.28	1.27	0.89	0.89
VI-c	3	343.26	0.5392	0.59	0.59	4.54	4.56	2.54	2.58
VI-c	4	318.25	0.5065	0.53	0.53	3.36	3.38	1.50	1.54
VI-c	5	315.18	0.3115	0.51	0.51	6.69	6.70	3.01	3.04
VI-c	6	287.24	0.0621	0.55	0.55	5.04	5.02	2.62	2.63
VI-d	1	568.81	0.2586	0.62	0.62	4.23	4.23	2.53	2.56
VI-d	2	322.10	0.5661	0.50	0.50	2.60	2.60	1.25	1.26
VI-d	3	312.13	0.1518	0.61	0.61	4.49	4.50	2.62	2.65
VI-d	4	306.79	0.0773	0.40	0.40	2.32	2.32	0.89	0.89
VI-d	5	295.10	0.0020	0.62	0.62	0.50	0.51	0.30	0.30
VI-d	6	287.20	0.0172	0.64	0.64	5.86	5.86	3.64	3.66

#	t	λ	f	$\tilde{\chi}$	$\tilde{\chi}^{\text{NTO}}$	$\tilde{\zeta}_{\pm}$	$\tilde{\zeta}_{\pm}^{\text{NTO}}$	ζ	ζ^{NTO}
VI-e	1	558.72	0.2970	0.59	0.59	3.96	3.95	2.28	2.29
VI-e	2	320.52	0.0019	0.70	0.69	1.58	1.60	1.06	1.07
VI-e	3	319.18	0.5542	0.51	0.51	2.86	2.86	1.44	1.45
VI-e	4	316.14	0.3039	0.56	0.56	0.74	0.74	0.41	0.41
VI-e	5	308.58	0.0797	0.49	0.49	5.02	5.03	2.39	2.42
VI-e	6	286.13	0.0603	0.45	0.45	4.78	4.78	2.13	2.14
VI-f	1	545.01	0.3291	0.58	0.58	3.86	3.85	2.14	2.15
VI-f	2	337.84	0.0030	0.70	0.70	1.44	1.44	0.99	1.00
VI-f	3	322.13	0.3916	0.54	0.54	4.28	4.29	2.27	2.28
VI-f	4	308.47	0.1447	0.39	0.39	3.90	3.89	1.43	1.44
VI-f	5	305.30	0.3482	0.59	0.59	2.82	2.82	1.54	1.56
VI-f	6	284.57	0.0978	0.47	0.47	5.36	5.36	2.41	2.43
VI-g	1	474.48	0.4499	0.47	0.47	2.79	2.79	1.20	1.22
VI-g	2	369.17	0.5428	0.56	0.56	3.46	3.47	1.76	1.79
VI-g	3	306.79	0.3490	0.57	0.57	3.78	3.77	2.07	2.08
VI-g	4	306.24	0.0064	0.70	0.70	1.92	1.92	1.31	1.31
VI-g	5	291.79	0.1637	0.48	0.48	1.84	1.85	0.85	0.87
VI-g	6	272.82	0.0391	0.58	0.58	3.63	3.62	2.06	2.06
VI-h	1	599.06	0.1308	0.59	0.58	5.00	5.01	2.76	2.81
VI-h	2	416.04	0.8953	0.53	0.53	4.51	4.51	2.29	2.32
VI-h	3	368.90	0.0009	0.72	0.72	0.13	0.12	0.09	0.09
VI-h	4	358.19	0.2945	0.62	0.62	8.86	8.85	5.39	5.41
VI-h	5	341.59	1.4826	0.41	0.41	0.85	0.86	0.34	0.35
VI-h	6	332.84	0.0171	0.45	0.45	1.14	1.13	0.51	0.51
VI-i	1	509.92	0.4129	0.54	0.54	3.32	3.32	1.71	1.73
VI-i	2	340.31	0.0013	0.72	0.71	1.73	1.73	1.20	1.21
VI-i	3	308.92	0.4154	0.57	0.57	3.67	3.67	2.01	2.02
VI-i	4	302.21	0.1482	0.43	0.43	0.19	0.18	0.09	0.09
VI-i	5	294.94	0.2030	0.47	0.47	3.59	3.61	1.64	1.66
VI-i	6	274.52	0.0727	0.37	0.37	4.47	4.48	1.59	1.61

#	t	λ	f	$\tilde{\chi}$	$\tilde{\chi}^{\text{NTO}}$	$\tilde{\zeta}_{\pm}$	$\tilde{\zeta}_{\pm}^{\text{NTO}}$	ζ	ζ^{NTO}
VI-j	1	505.02	0.4207	0.54	0.54	3.32	3.32	1.70	1.72
VI-j	2	341.28	0.0011	0.73	0.73	2.55	2.55	1.83	1.84
VI-j	3	308.26	0.3804	0.55	0.55	3.48	3.48	1.86	1.87
VI-j	4	307.33	0.2809	0.56	0.56	3.23	3.23	1.78	1.80
VI-j	5	294.51	0.1048	0.44	0.43	3.22	3.23	1.34	1.35
VI-j	6	288.51	0.0098	0.81	0.81	5.43	5.43	4.34	4.35
VI-n	1	695.01	0.1777	0.63	0.63	4.24	4.24	2.59	2.62
VI-n	2	367.61	0.1872	0.55	0.55	7.69	7.71	4.12	4.16
VI-n	3	341.91	0.0012	0.69	0.69	0.78	0.79	0.52	0.52
VI-n	4	334.30	0.0557	0.68	0.69	3.52	3.52	2.40	2.40
VI-n	5	330.36	0.6836	0.47	0.47	1.58	1.59	0.72	0.73
VI-n	6	317.18	0.0388	0.72	0.72	3.55	3.54	2.51	2.51
VI-o	1	527.66	0.7065	0.51	0.51	2.63	2.62	1.30	1.30
VI-o	2	354.82	0.0016	0.71	0.71	1.92	1.91	1.35	1.35
VI-o	3	326.30	0.6037	0.59	0.59	3.63	3.64	2.12	2.14
VI-o	4	314.06	0.0113	0.43	0.43	1.98	1.98	0.83	0.84
VI-o	5	302.21	0.1537	0.56	0.56	0.19	0.18	0.12	0.11
VI-o	6	290.26	0.0512	0.39	0.39	2.95	2.95	1.11	1.12
VI-p	1	673.55	0.1734	0.64	0.64	4.51	4.50	2.81	2.84
VI-p	2	427.75	0.1872	0.72	0.72	9.05	9.06	6.38	6.41
VI-p	3	336.50	0.6281	0.51	0.51	4.48	4.49	2.25	2.27
VI-p	4	332.39	0.0453	0.72	0.72	4.13	4.13	2.94	2.95
VI-p	5	320.28	0.0055	0.65	0.65	0.19	0.20	0.12	0.13
VI-p	6	317.67	0.0198	0.70	0.70	3.63	3.63	2.48	2.49
VI-q	1	546.80	0.9406	0.50	0.50	1.64	1.63	0.79	0.80
VI-q	2	365.51	0.0131	0.61	0.61	0.22	0.21	0.13	0.13
VI-q	3	359.65	0.3921	0.66	0.66	2.99	2.99	1.95	1.96
VI-q	4	359.33	0.0013	0.72	0.72	2.25	2.26	1.60	1.60
VI-q	5	309.36	0.0827	0.52	0.52	0.93	0.93	0.46	0.47
VI-q	6	301.44	0.0228	0.51	0.51	2.30	2.31	1.15	1.17

#	t	λ	f	$\tilde{\chi}$	$\tilde{\chi}^{\text{NTO}}$	$\tilde{\zeta}_{\pm}$	$\tilde{\zeta}_{\pm}^{\text{NTO}}$	ζ	ζ^{NTO}
VI-r	1	465.62	0.5066	0.48	0.48	3.06	3.07	1.41	1.43
VI-r	2	330.30	0.4624	0.53	0.53	2.03	2.03	1.03	1.05
VI-r	3	302.63	0.3155	0.60	0.60	4.60	4.61	2.72	2.73
VI-r	4	287.20	0.0012	0.73	0.73	0.88	0.89	0.64	0.64
VI-r	5	286.09	0.1429	0.43	0.43	2.28	2.29	0.95	0.97
VI-r	6	264.97	0.0112	0.47	0.47	3.09	3.09	1.42	1.43
VI-s	1	655.04	0.4127	0.59	0.59	3.95	3.96	2.21	2.25
VI-s	2	359.57	0.0597	0.68	0.68	3.23	3.23	2.16	2.18
VI-s	3	351.07	0.5950	0.54	0.54	3.20	3.21	1.65	1.67
VI-s	4	345.64	0.0020	0.70	0.70	1.39	1.38	0.95	0.95
VI-s	5	312.93	0.0061	0.39	0.39	3.46	3.47	1.31	1.32
VI-s	6	291.82	0.0000	0.84	0.84	0.93	0.93	0.76	0.76
VI-t	1	699.38	0.4786	0.59	0.59	3.96	3.98	2.25	2.29
VI-t	2	384.05	0.0525	0.69	0.70	3.15	3.15	2.17	2.19
VI-t	3	363.43	0.7127	0.55	0.55	3.19	3.20	1.70	1.72
VI-t	4	345.04	0.0019	0.70	0.70	1.37	1.38	0.93	0.94
VI-t	5	320.37	0.0198	0.43	0.43	3.46	3.47	1.47	1.48
VI-t	6	301.77	0.0009	0.86	0.86	0.34	0.34	0.29	0.29
VI-u	1	1064.39	0.2281	0.61	0.61	4.43	4.43	2.64	2.67
VI-u	2	465.95	0.2176	0.64	0.64	5.51	5.52	3.43	3.47
VI-u	3	440.78	0.0946	0.57	0.57	7.17	7.18	4.04	4.07
VI-u	4	392.15	1.0324	0.50	0.50	1.27	1.28	0.63	0.64
VI-u	5	337.94	0.0011	0.68	0.68	0.75	0.76	0.49	0.50
VI-u	6	314.22	0.0463	0.64	0.64	3.84	3.83	2.42	2.43
VI-v	1	1062.43	0.2043	0.60	0.60	4.65	4.65	2.73	2.76
VI-v	2	613.85	0.2649	0.70	0.70	9.08	9.10	6.19	6.26
VI-v	3	456.01	0.0288	0.70	0.70	4.75	4.75	3.31	3.33
VI-v	4	412.25	0.8912	0.57	0.57	5.34	5.35	3.00	3.02
VI-v	5	376.95	0.2167	0.74	0.74	9.09	9.09	6.63	6.66
VI-v	6	350.34	0.0405	0.66	0.66	8.25	8.25	5.37	5.37

#	t	λ	f	$\tilde{\chi}$	$\tilde{\chi}^{\text{NTO}}$	$\tilde{\zeta}_{\pm}$	$\tilde{\zeta}_{\pm}^{\text{NTO}}$	ζ	ζ^{NTO}
VII	1	663.38	0.3530	0.55	0.55	3.88	3.90	2.06	2.09
VII	2	330.09	0.5669	0.51	0.51	2.97	2.97	1.47	1.48
VII	3	315.86	0.0773	0.70	0.70	2.86	2.86	1.97	1.98
VII	4	303.44	0.0860	0.52	0.52	1.75	1.74	0.90	0.90
VII	5	291.18	0.0034	0.80	0.80	2.24	2.23	1.78	1.78
VII	6	283.49	0.2059	0.60	0.60	2.09	2.09	1.24	1.24
VIII	1	561.52	0.0465	0.58	0.57	5.55	5.55	3.06	3.12
VIII	2	423.09	0.0005	0.72	0.72	0.52	0.51	0.37	0.36
VIII	3	345.57	0.6689	0.49	0.49	1.55	1.55	0.74	0.75
VIII	4	295.17	0.0000	0.76	0.76	2.25	2.26	1.63	1.65
VIII	5	281.71	0.0210	0.51	0.51	1.37	1.37	0.70	0.70
VIII	6	247.11	0.0319	0.54	0.54	4.69	4.70	2.52	2.53
IX-a	1	1057.32	0.1209	0.66	0.66	6.32	6.35	4.01	4.09
IX-a	2	432.71	0.0003	0.71	0.72	0.21	0.21	0.17	0.17
IX-a	3	379.22	0.5883	0.46	0.45	3.15	3.15	1.40	1.41
IX-a	4	376.92	0.1915	0.72	0.73	4.72	4.72	3.38	3.40
IX-a	5	355.92	0.1925	0.57	0.57	4.49	4.49	2.54	2.57
IX-a	6	345.15	0.0037	0.80	0.80	4.40	4.40	3.50	3.51
IX-b	1	2181.38	0.0968	0.70	0.68	6.78	6.80	4.33	4.45
IX-b	2	551.88	0.0673	0.74	0.74	6.10	6.11	4.51	4.55
IX-b	3	451.56	0.8685	0.49	0.49	3.55	3.57	1.67	1.71
IX-b	4	430.33	0.0003	0.72	0.72	0.36	0.40	0.25	0.29
IX-b	5	383.48	0.0077	0.58	0.58	5.28	5.28	3.01	3.05
IX-b	6	355.34	0.3972	0.53	0.53	2.11	2.11	1.09	1.10
X	1	717.37	0.1809	0.51	0.51	6.68	6.71	3.07	3.21
X	2	380.35	0.3580	0.48	0.48	1.93	1.93	0.87	0.89
X	3	338.35	0.0346	0.43	0.43	2.76	2.76	1.13	1.14
X	4	329.05	0.3910	0.47	0.47	0.80	0.81	0.34	0.34
X	5	304.88	0.0479	0.61	0.61	5.78	5.78	3.15	3.19
X	6	296.30	0.3412	0.44	0.44	0.47	0.46	0.19	0.20

#	t	λ	f	$\tilde{\chi}$	$\tilde{\chi}^{\text{NTO}}$	$\tilde{\zeta}_{\pm}$	$\tilde{\zeta}_{\pm}^{\text{NTO}}$	ζ	ζ^{NTO}
XI	1	1429.86	0.0828	0.70	0.69	6.38	6.41	4.23	4.32
XI	2	434.18	0.0826	0.77	0.77	5.94	5.94	4.53	4.55
XI	3	413.34	0.0004	0.71	0.71	0.33	0.34	0.25	0.25
XI	4	374.67	0.5616	0.51	0.51	4.10	4.12	2.04	2.06
XI	5	353.92	0.4041	0.52	0.52	3.19	3.21	1.62	1.65
XI	6	339.78	0.0075	0.62	0.62	5.07	5.07	3.13	3.15
XII	1	484.21	0.2219	0.48	0.48	3.14	3.12	1.43	1.44
XII	2	358.94	0.3741	0.73	0.73	9.82	9.83	7.00	7.05
XII	3	356.32	0.4517	0.58	0.58	7.36	7.36	4.17	4.20
XII	4	306.05	0.1502	0.50	0.50	2.53	2.52	1.21	1.22
XII	5	303.73	0.7361	0.53	0.53	0.71	0.71	0.36	0.36
XII	6	288.21	0.0855	0.50	0.50	2.05	2.06	0.99	1.01

As expected, we see that there is a linear correlation between NTOs and Detachment/Attachment-derived quantities values:

$f^{\text{NTO}} = af^{\text{D/A}} + b$				
f^{NTO}	$f^{\text{D/A}}$	a	b	R^2
$\tilde{\chi}^{\text{NTO}}$	$\tilde{\chi}$	0.99952	- 0.00013	1.000
$\tilde{\zeta}_{\pm}^{\text{NTO}}$	$\tilde{\zeta}_{\pm}$	1.00101	- 0.00065	1.000
ζ^{NTO}	ζ	1.00678	+0.00270	1.000