



Supporting Information

for

Experimental and computational electrochemistry of quinazolinespirohexadienone molecular switches – differential electrochromic vs photochromic behavior

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Additional figures and Z-matrices

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Excel Spreadsheet with <u>all</u> Experimental and Computational E_{red}^0 Data	separate file

Figure S1: Frontier molecular orbitals for **1b** and **3b**, cf. Figure 6 (for **1a**). HOMO (MO 97 for **1b**, 101 for **3b**) in red/blue; LUMO (MO 98 for **1b**, 102 for **3b**) in green/yellow.

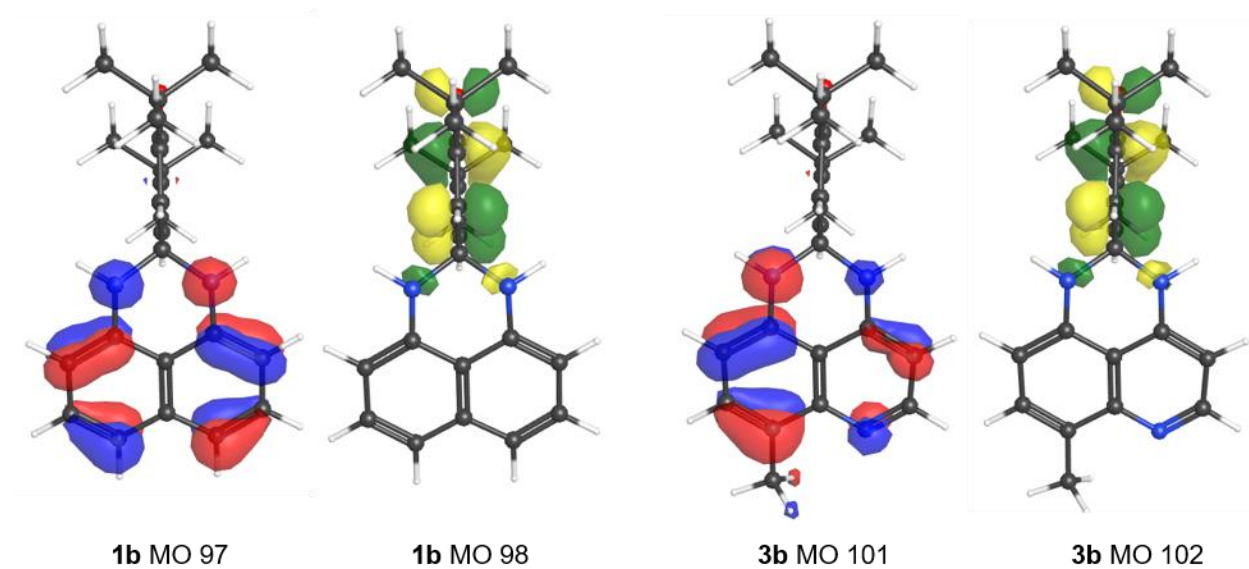


Figure S2: Geometry visualizations for **3a** S_0 , T_0 , D_0 (Z-matrices in Figures S3–S5).

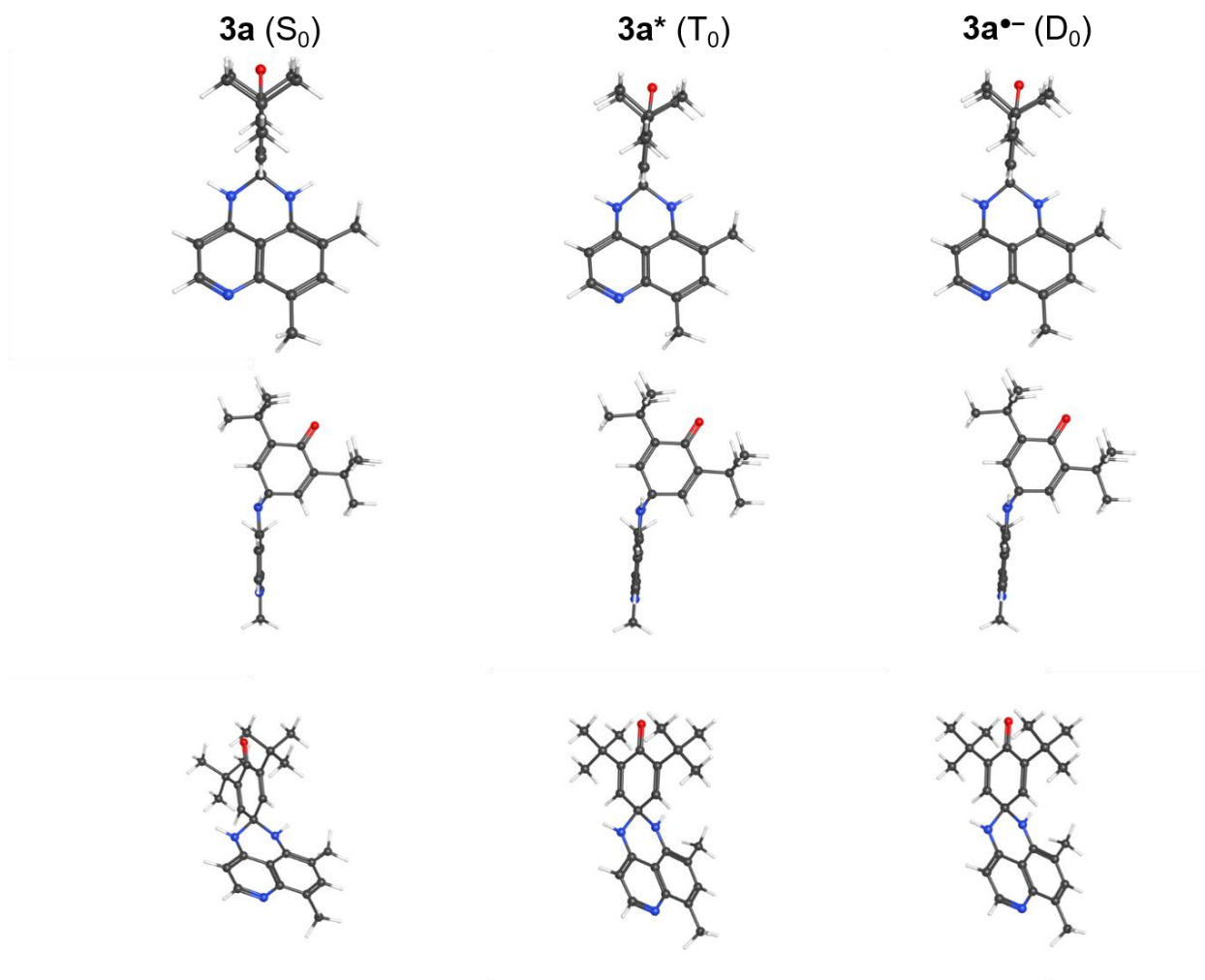


Figure S3: Z-matrix for 3a S₀ geometry

C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1
C	4	B4	3	A3	2	D2
C	5	B5	4	A4	3	D3
C	2	B6	3	A5	4	D4
N	7	B7	2	A6	3	D5
C	8	B8	7	A7	2	D6
C	9	B9	8	A8	7	D7
C	6	B10	7	A9	2	D8
N	11	B11	6	A10	7	D9
C	12	B12	11	A11	6	D10
N	5	B13	4	A12	3	D11
H	14	B14	5	A13	4	D12
C	13	B15	12	A14	11	D13
C	16	B16	13	A15	12	D14
C	17	B17	16	A16	13	D15
C	18	B18	17	A17	16	D16
C	19	B19	18	A18	17	D17
H	20	B20	19	A19	18	D18
C	19	B21	18	A20	17	D19
C	22	B22	19	A21	18	D20
H	23	B23	22	A22	19	D21
H	23	B24	22	A23	19	D22
H	23	B25	22	A24	19	D23
C	22	B26	19	A25	18	D24
H	27	B27	22	A26	19	D25
H	27	B28	22	A27	19	D26
H	27	B29	22	A28	19	D27
C	22	B30	19	A29	18	D28
H	31	B31	22	A30	19	D29
H	31	B32	22	A31	19	D30
H	31	B33	22	A32	19	D31
O	18	B34	17	A33	16	D32
C	17	B35	16	A34	13	D33
C	36	B36	17	A35	16	D34
H	37	B37	36	A36	17	D35
H	37	B38	36	A37	17	D36
H	37	B39	36	A38	17	D37
C	36	B40	17	A39	16	D38
H	41	B41	36	A40	17	D39
H	41	B42	36	A41	17	D40
H	41	B43	36	A42	17	D41
C	36	B44	17	A43	16	D42
H	45	B45	36	A44	17	D43
H	45	B46	36	A45	17	D44
H	45	B47	36	A46	17	D45
H	16	B48	13	A47	12	D46
H	12	B49	11	A48	6	D47

H	10	B50	11	A49	6	D48
H	9	B51	10	A50	11	D49
C	4	B52	5	A51	6	D50
H	53	B53	4	A52	5	D51
H	53	B54	4	A53	5	D52
H	53	B55	4	A54	5	D53
H	3	B56	4	A55	5	D54
H	1	B57	2	A56	3	D55
H	1	B58	2	A57	3	D56
H	1	B59	2	A58	3	D57

B1 1.507714864
 B2 1.384706967
 B3 1.415486447
 B4 1.392744841
 B5 1.421360869
 B6 1.427154868
 B7 1.368964415
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 B31 1.096628923
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D53 59.40065809
D54 -179.8142697
D55 0.421590815
D56 121.0026485
D57 -120.1664666

Figure S4: Z-matrix for 3a* T₀ geometry

C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1
C	4	B4	3	A3	2	D2
C	5	B5	4	A4	3	D3
C	2	B6	3	A5	4	D4
N	7	B7	2	A6	3	D5
C	8	B8	7	A7	2	D6
C	9	B9	8	A8	7	D7
C	6	B10	7	A9	2	D8
N	11	B11	6	A10	7	D9
C	12	B12	11	A11	6	D10
N	5	B13	4	A12	3	D11
H	14	B14	5	A13	4	D12
C	13	B15	12	A14	11	D13
C	16	B16	13	A15	12	D14
C	17	B17	16	A16	13	D15
C	18	B18	17	A17	16	D16
C	19	B19	18	A18	17	D17
H	20	B20	19	A19	18	D18
C	19	B21	18	A20	17	D19
C	22	B22	19	A21	18	D20
H	23	B23	22	A22	19	D21
H	23	B24	22	A23	19	D22
H	23	B25	22	A24	19	D23
C	22	B26	19	A25	18	D24
H	27	B27	22	A26	19	D25
H	27	B28	22	A27	19	D26
H	27	B29	22	A28	19	D27
C	22	B30	19	A29	18	D28
H	31	B31	22	A30	19	D29
H	31	B32	22	A31	19	D30
H	31	B33	22	A32	19	D31
O	18	B34	17	A33	16	D32
C	17	B35	16	A34	13	D33
C	36	B36	17	A35	16	D34
H	37	B37	36	A36	17	D35
H	37	B38	36	A37	17	D36
H	37	B39	36	A38	17	D37
C	36	B40	17	A39	16	D38
H	41	B41	36	A40	17	D39
H	41	B42	36	A41	17	D40
H	41	B43	36	A42	17	D41
C	36	B44	17	A43	16	D42
H	45	B45	36	A44	17	D43
H	45	B46	36	A45	17	D44
H	45	B47	36	A46	17	D45
H	16	B48	13	A47	12	D46
H	12	B49	11	A48	6	D47

H	10	B50	11	A49	6	D48
H	9	B51	10	A50	11	D49
C	4	B52	5	A51	6	D50
H	53	B53	4	A52	5	D51
H	53	B54	4	A53	5	D52
H	53	B55	4	A54	5	D53
H	3	B56	4	A55	5	D54
H	1	B57	2	A56	3	D55
H	1	B58	2	A57	3	D56
H	1	B59	2	A58	3	D57

B1 1.497699881
 B2 1.400954065
 B3 1.392470012
 B4 1.438856168
 B5 1.427144140
 B6 1.443339376
 B7 1.351240087
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 B36 1.548629436
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D14 -130.6714857
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D16 2.755064955
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D20 -179.1289578
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D28 -59.41377415

D29 178.8006567
D30 -62.23414336
D31 58.28219182
D32 -178.2723737
D33 -179.3719086
D34 -120.7409455
D35 62.37521503
D36 -178.6736445
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D39 -60.55622385
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D41 -179.5609160
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D43 58.48133577
D44 179.0305199
D45 -61.97709265
D46 50.53367599
D47 -174.3370818
D48 179.9687080
D49 179.5408735
D50 179.5650747
D51 -179.5733987
D52 -59.48237068
D53 60.43781312
D54 -179.4915275
D55 0.349819572
D56 121.5218253
D57 -120.9121702

Figure S5: Z-matrix for **3a⁺** D₀ geometry

C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1
C	4	B4	3	A3	2	D2
C	5	B5	4	A4	3	D3
C	2	B6	3	A5	4	D4
N	7	B7	2	A6	3	D5
C	8	B8	7	A7	2	D6
C	9	B9	8	A8	7	D7
C	6	B10	7	A9	2	D8
N	11	B11	6	A10	7	D9
C	12	B12	11	A11	6	D10
N	5	B13	4	A12	3	D11
H	14	B14	5	A13	4	D12
C	13	B15	12	A14	11	D13
C	16	B16	13	A15	12	D14
C	17	B17	16	A16	13	D15
C	18	B18	17	A17	16	D16
C	19	B19	18	A18	17	D17
H	20	B20	19	A19	18	D18
C	19	B21	18	A20	17	D19
C	22	B22	19	A21	18	D20
H	23	B23	22	A22	19	D21
H	23	B24	22	A23	19	D22
H	23	B25	22	A24	19	D23
C	22	B26	19	A25	18	D24
H	27	B27	22	A26	19	D25
H	27	B28	22	A27	19	D26
H	27	B29	22	A28	19	D27
C	22	B30	19	A29	18	D28
H	31	B31	22	A30	19	D29
H	31	B32	22	A31	19	D30
H	31	B33	22	A32	19	D31
O	18	B34	17	A33	16	D32
C	17	B35	16	A34	13	D33
C	36	B36	17	A35	16	D34
H	37	B37	36	A36	17	D35
H	37	B38	36	A37	17	D36
H	37	B39	36	A38	17	D37
C	36	B40	17	A39	16	D38
H	41	B41	36	A40	17	D39
H	41	B42	36	A41	17	D40
H	41	B43	36	A42	17	D41
C	36	B44	17	A43	16	D42
H	45	B45	36	A44	17	D43
H	45	B46	36	A45	17	D44
H	45	B47	36	A46	17	D45
H	16	B48	13	A47	12	D46
H	12	B49	11	A48	6	D47

H	10	B50	11	A49	6	D48
H	9	B51	10	A50	11	D49
C	4	B52	5	A51	6	D50
H	53	B53	4	A52	5	D51
H	53	B54	4	A53	5	D52
H	53	B55	4	A54	5	D53
H	3	B56	4	A55	5	D54
H	1	B57	2	A56	3	D55
H	1	B58	2	A57	3	D56
H	1	B59	2	A58	3	D57

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