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

Electronic Supplementary Information

An experimental NEXAFS and computational TDDFT and ΔDFT study of the gas-phase core excitation spectra of nitroxide free radical TEMPO and its analogues

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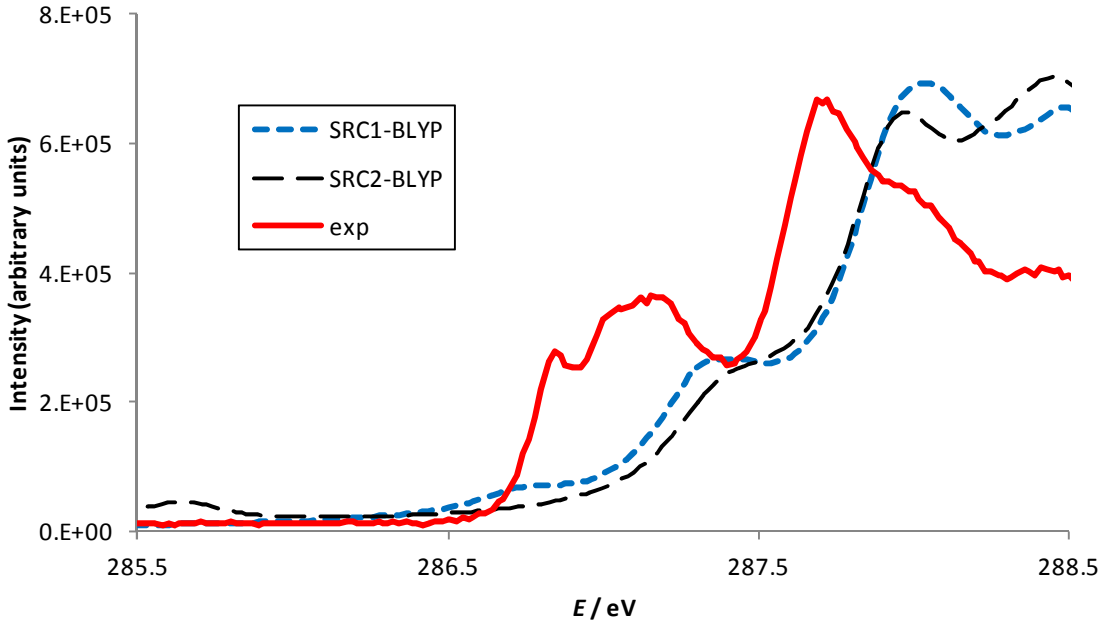

Figure S1. The experimental and modelled C1s core-excited spectrum of **tempo**. The relative overlap is calculated for the 285.6–288.8 eV (285.0–288.7 eV) region for SRC1 (SRC2).

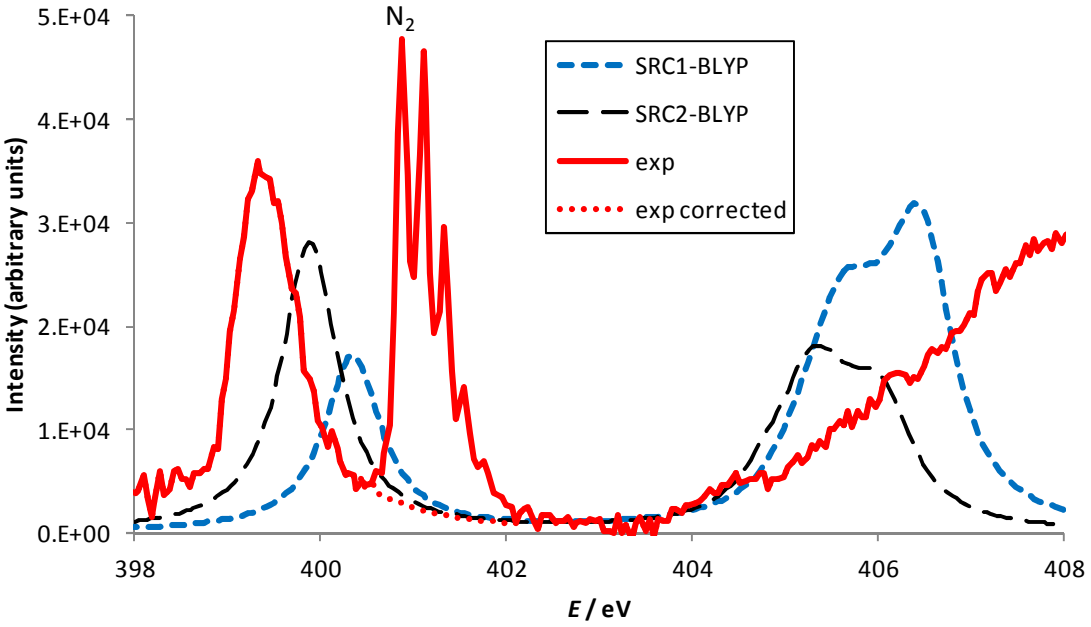

Figure S2. The experimental and modelled N1s core-excited spectrum of **tempo**. The relative overlap is calculated for the 398.0–406.5 eV (398.0–406.2 eV) region for SRC1 (SRC2). The experimental spectrum is corrected (exp corrected) for the presence of N_2.

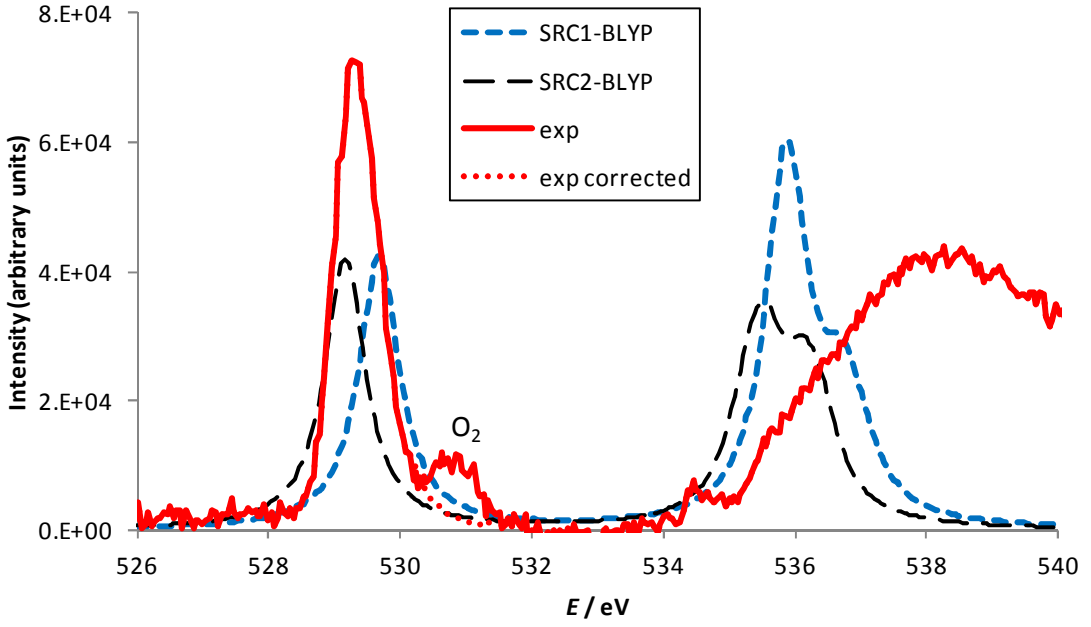

Figure S3. The experimental and modelled O1s core-excited spectrum of **tempo**. The relative overlap is calculated for the 527.0–537.2 eV (527.0–536.5 eV) region for SRC1 (SRC2).The experimental spectrum is corrected (exp corrected) for the presence of O_2.

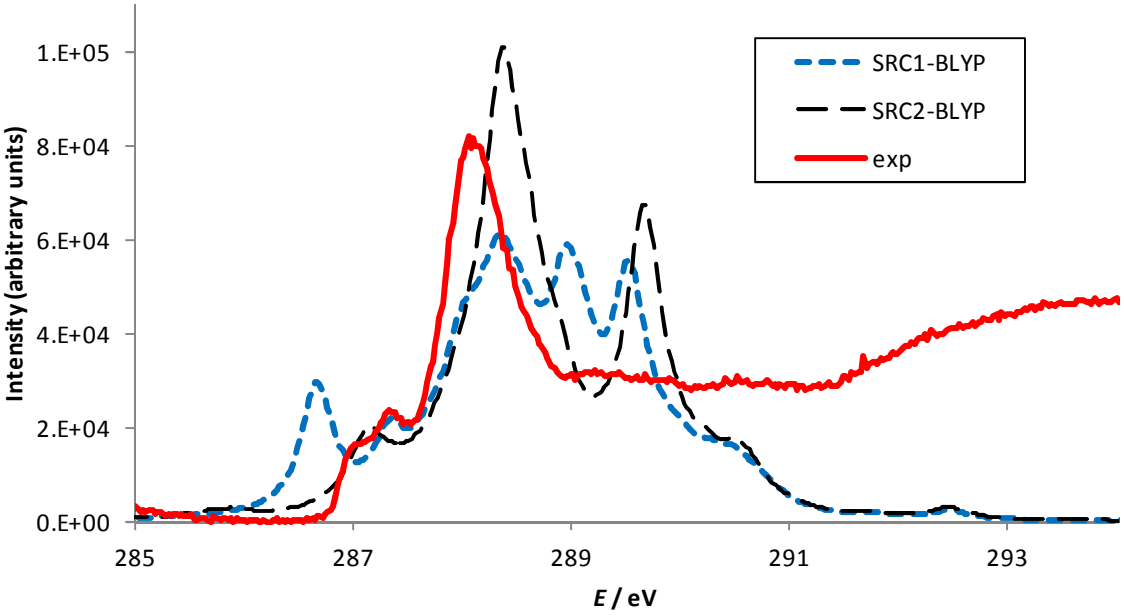

Figure S4. The experimental and modelled C1s core-excited spectrum of **nit8**. The relative overlap is calculated for the 285.5–288.7 eV (285.5–288.5 eV) region for SRC1 (SRC2).

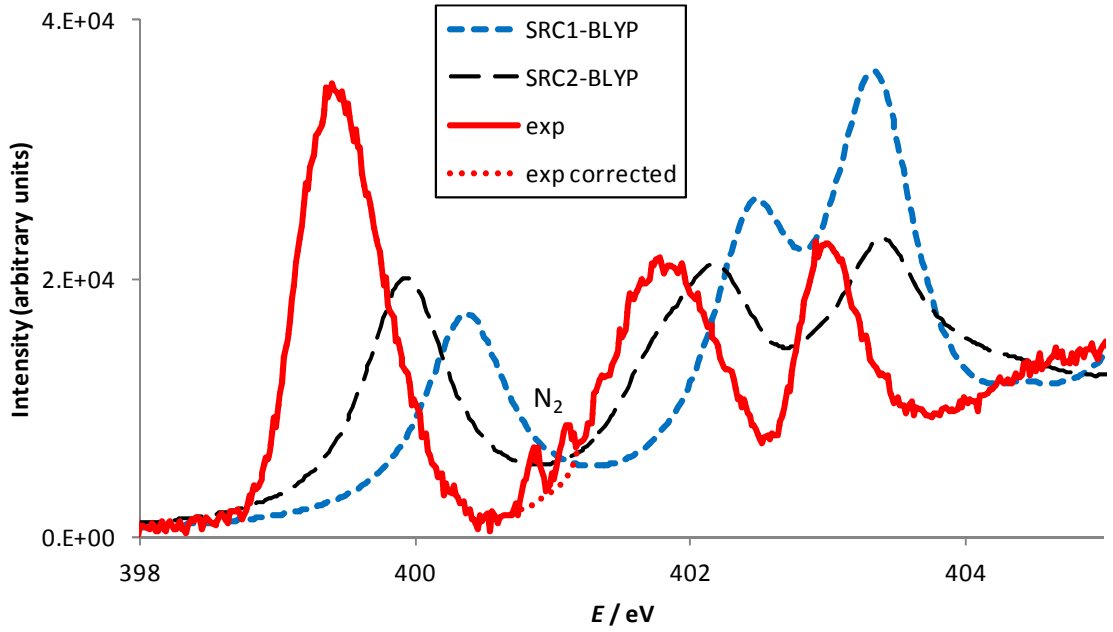

Figure S5. The experimental and modelled N1s core-excited spectrum of **nit8**. The relative overlap is calculated for the 398.0–405.2 eV (398.0–405.2 eV) region for SRC1 (SRC2). The experimental spectrum is corrected (exp corrected) for the presence of N_2.

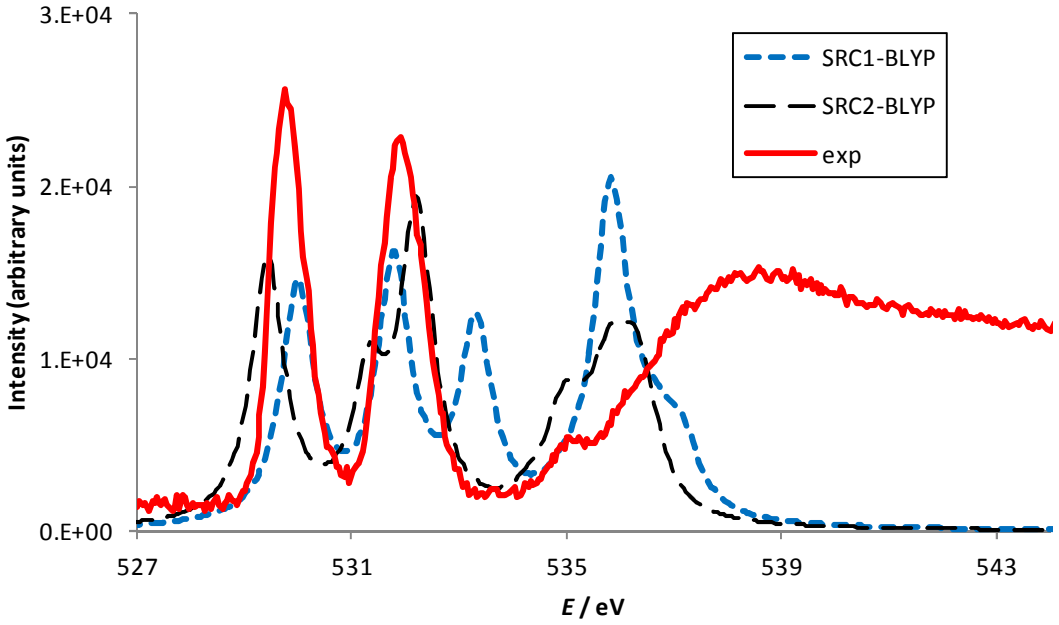

Figure S6. The experimental and modelled O1s core-excited spectrum of **nit8**. The relative overlap is calculated for the 527.0–536.7 eV (527.0–536.3 eV) region for SRC1 (SRC2).

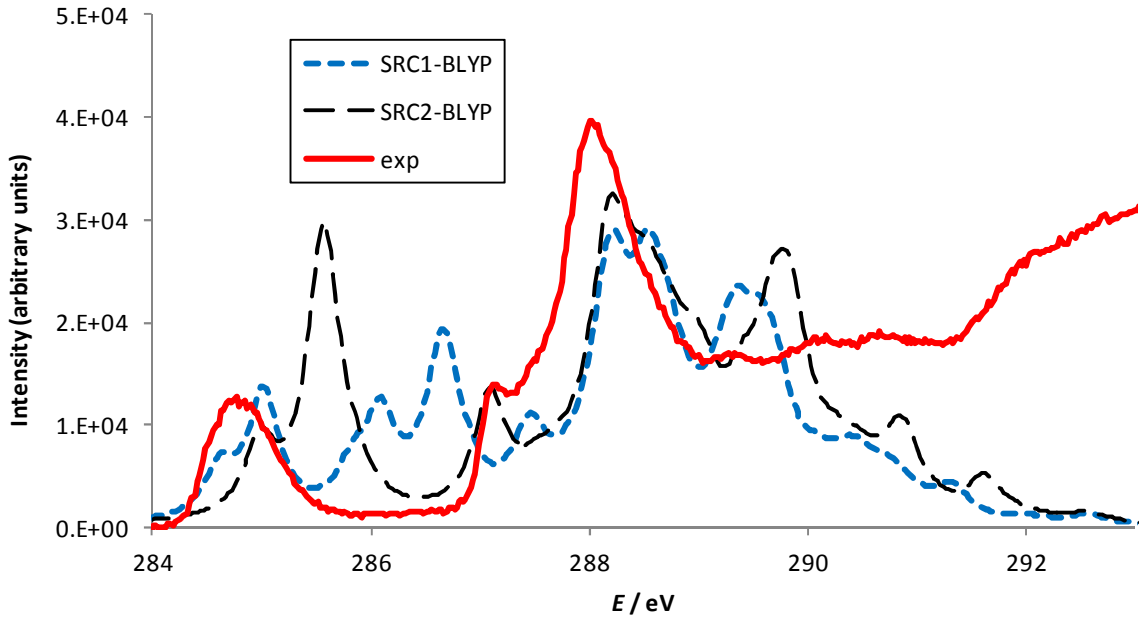

Figure S7. The experimental and modelled C1s core-excited spectrum of **nit9**. The relative overlap is calculated for the 284.0–288.8 eV (284.0–288.6 eV) region for SRC1 (SRC2).

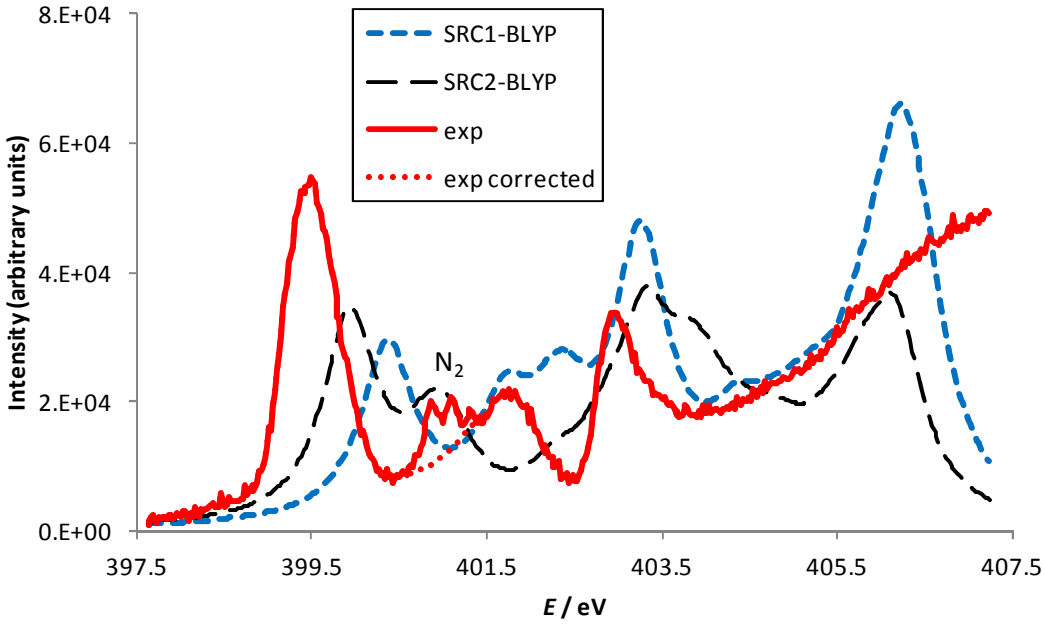

Figure S8. The experimental and modelled N1s core-excited spectrum of **nit9**. The relative overlap is calculated for the 397.6–405.4 eV (397.6–405.1 eV) region for SRC1 (SRC2). The experimental spectrum is corrected (exp corrected) for the presence of N_2.

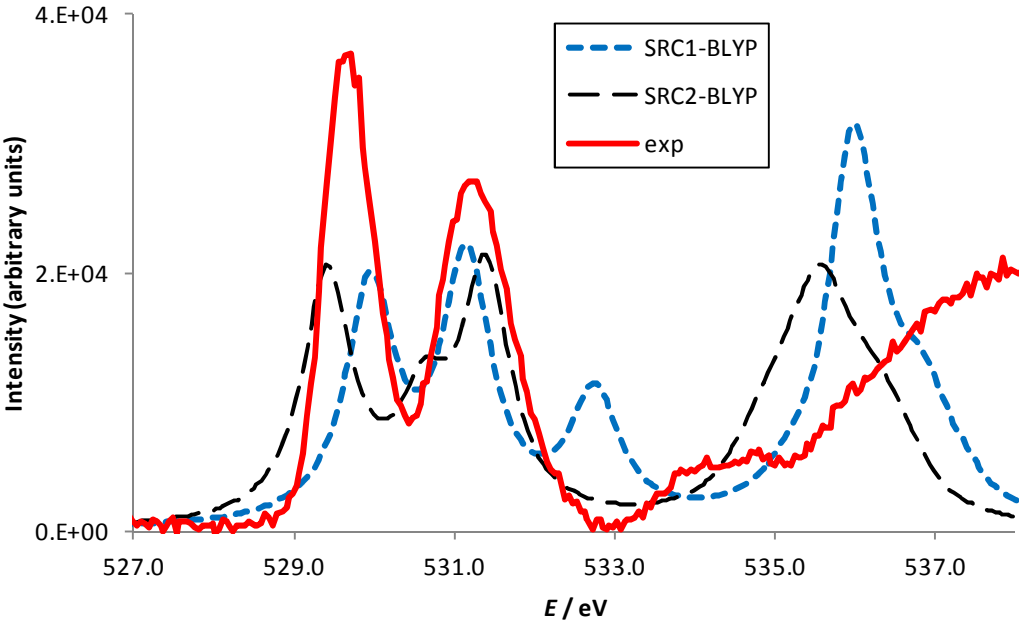

Figure S9. The experimental and modelled O1s core-excited spectrum of **nit9**. The relative overlap is calculated for the 527.0–536.9 eV (527.0–536.4 eV) region for SRC1 (SRC2).

Table S1: tempo C1s excitation energies (in eV) and oscillator strengths at the TDDFT-BLYP-SRC1/6-311(2+)G* level.

C1		C2		C3		C4		C5	
288.09	0.0003	288.09	0.0001	287.40	0.0000	287.32	0.0000	287.36	0.0001
289.46	0.0003	289.46	0.0002	287.90	0.0013	287.96	0.0011	287.91	0.0007
289.51	0.0000	289.50	0.0000	288.06	0.0011	288.10	0.0008	288.03	0.0007
289.86	0.0000	289.86	0.0000	288.46	0.0032	288.47	0.0006	288.46	0.0001
289.88	0.0061	289.88	0.0035	288.55	0.0001	288.49	0.0004	288.52	0.0005
289.89	0.0030	289.89	0.0017	288.60	0.0013	288.57	0.0003	288.56	0.0008
289.90	0.0000	289.90	0.0000	288.60	0.0001	288.61	0.0001	288.59	0.0001
289.95	0.0000	289.95	0.0001	288.66	0.0002	288.73	0.0002	288.66	0.0005
290.04	0.0001	290.04	0.0000	288.74	0.0001	288.76	0.0001	288.74	0.0001
290.11	0.0042	290.11	0.0040	289.01	0.0004	288.96	0.0002	288.99	0.0012
290.35	0.0001	290.35	0.0001	289.09	0.0001	289.07	0.0001	289.07	0.0003
290.39	0.0015	290.39	0.0012	289.18	0.0003	289.15	0.0006	289.16	0.0000
290.45	0.0006	290.45	0.0004	289.20	0.0000	289.17	0.0005	289.18	0.0001
290.46	0.0001	290.46	0.0000	289.20	0.0007	289.20	0.0001	289.20	0.0000
290.50	0.0002	290.50	0.0002	289.21	0.0000	289.21	0.0002	289.20	0.0007
290.50	0.0001	290.50	0.0001	289.23	0.0000	289.24	0.0000	289.21	0.0001
290.55	0.0013	290.55	0.0007	289.28	0.0001	289.28	0.0002	289.27	0.0001
290.56	0.0000	290.56	0.0000	289.30	0.0000	289.29	0.0000	289.28	0.0006
290.61	0.0000	290.61	0.0000	289.34	0.0000	289.34	0.0000	289.32	0.0003
290.70	0.0051	290.70	0.0033	289.36	0.0006	289.38	0.0005	289.35	0.0001

C6		C7		C8		C9	
286.74	0.0013	286.74	0.0004	286.69	0.0002	286.69	0.0002
287.47	0.0033	287.47	0.0023	287.31	0.0052	287.31	0.0053
287.76	0.0012	287.76	0.0006	287.67	0.0009	287.67	0.0009
288.05	0.0068	288.05	0.0065	287.92	0.0091	287.92	0.0101
288.19	0.0016	288.19	0.0014	287.97	0.0009	287.97	0.0010
288.24	0.0005	288.24	0.0003	288.07	0.0004	288.07	0.0005
288.30	0.0006	288.30	0.0002	288.15	0.0037	288.15	0.0039
288.32	0.0036	288.32	0.0027	288.19	0.0002	288.19	0.0003
288.42	0.0002	288.42	0.0001	288.27	0.0001	288.27	0.0001
288.53	0.0023	288.53	0.0039	288.36	0.0031	288.36	0.0027
288.71	0.0029	288.71	0.0029	288.51	0.0066	288.51	0.0065
288.72	0.0013	288.72	0.0011	288.58	0.0003	288.58	0.0002
288.77	0.0009	288.77	0.0008	288.60	0.0001	288.60	0.0001
288.83	0.0001	288.83	0.0001	288.67	0.0000	288.67	0.0000
288.87	0.0001	288.87	0.0001	288.72	0.0001	288.72	0.0001
288.88	0.0003	288.88	0.0001	288.75	0.0006	288.75	0.0006
288.93	0.0001	288.93	0.0000	288.77	0.0007	288.76	0.0008
288.96	0.0003	288.96	0.0002	288.80	0.0000	288.80	0.0000
288.99	0.0004	288.98	0.0003	288.83	0.0001	288.83	0.0002
288.99	0.0009	288.99	0.0006	288.84	0.0017	288.84	0.0018

Table S2: tempo C1s excitation energies (in eV) and oscillator strengths at the TDDFT-BLYP-SRC2/6-311(2+)G* level.

C1		C2		C3		C4		C5	
287.30	0.0002	287.30	0.0001	286.21	0.0001	286.20	0.0000	286.23	0.0000
289.36	0.0020	289.36	0.0015	287.88	0.0004	287.88	0.0006	287.75	0.0014
289.42	0.0000	289.42	0.0000	287.96	0.0016	287.96	0.0015	287.91	0.0014
289.67	0.0186	289.68	0.0143	288.39	0.0003	288.37	0.0003	288.30	0.0027
289.81	0.0001	289.81	0.0001	288.41	0.0018	288.41	0.0001	288.43	0.0004
289.83	0.0000	289.83	0.0000	288.44	0.0006	288.43	0.0005	288.44	0.0004
289.85	0.0003	289.85	0.0005	288.47	0.0028	288.47	0.0001	288.45	0.0005
289.89	0.0000	289.89	0.0001	288.59	0.0000	288.60	0.0003	288.49	0.0003
289.98	0.0002	289.98	0.0000	288.61	0.0001	288.62	0.0002	288.57	0.0005
290.01	0.0022	290.01	0.0025	288.83	0.0012	288.82	0.0002	288.86	0.0008
290.25	0.0004	290.25	0.0004	288.89	0.0006	288.88	0.0001	288.90	0.0004
290.35	0.0026	290.35	0.0025	289.06	0.0004	289.05	0.0004	289.05	0.0022
290.43	0.0002	290.43	0.0001	289.08	0.0002	289.07	0.0003	289.06	0.0001
290.43	0.0009	290.43	0.0008	289.08	0.0001	289.08	0.0003	289.07	0.0000
290.47	0.0001	290.47	0.0001	289.10	0.0001	289.10	0.0003	289.09	0.0001
290.48	0.0010	290.48	0.0006	289.14	0.0003	289.14	0.0000	289.10	0.0001
290.50	0.0034	290.50	0.0029	289.16	0.0003	289.16	0.0000	289.14	0.0003
290.53	0.0000	290.53	0.0001	289.18	0.0002	289.18	0.0002	289.18	0.0004
290.58	0.0000	290.58	0.0001	289.21	0.0001	289.21	0.0000	289.20	0.0003
290.59	0.0032	290.59	0.0029	289.27	0.0003	289.28	0.0005	289.22	0.0006

C6		C7		C8		C9	
285.65	0.0011	285.65	0.0006	285.58	0.0003	285.58	0.0002
287.41	0.0014	287.41	0.0011	287.34	0.0021	287.34	0.0021
287.59	0.0016	287.59	0.0011	287.49	0.0011	287.49	0.0011
287.94	0.0031	287.94	0.0029	287.77	0.0007	287.77	0.0008
288.01	0.0024	288.01	0.0022	287.87	0.0010	287.87	0.0012
288.03	0.0010	288.03	0.0008	287.91	0.0032	287.91	0.0036
288.10	0.0010	288.10	0.0006	287.99	0.0003	287.99	0.0005
288.19	0.0013	288.19	0.0011	288.03	0.0006	288.03	0.0006
288.22	0.0004	288.22	0.0003	288.07	0.0001	288.07	0.0002
288.36	0.0027	288.36	0.0036	288.21	0.0036	288.21	0.0034
288.49	0.0005	288.49	0.0008	288.35	0.0005	288.35	0.0005
288.60	0.0027	288.60	0.0024	288.46	0.0004	288.46	0.0003
288.64	0.0019	288.64	0.0017	288.48	0.0036	288.48	0.0036
288.66	0.0004	288.66	0.0004	288.50	0.0001	288.50	0.0001
288.70	0.0003	288.70	0.0003	288.56	0.0003	288.56	0.0002
288.73	0.0003	288.73	0.0001	288.60	0.0005	288.60	0.0005
288.76	0.0003	288.75	0.0002	288.62	0.0001	288.62	0.0001
288.80	0.0002	288.80	0.0002	288.62	0.0008	288.62	0.0009
288.82	0.0003	288.82	0.0002	288.66	0.0002	288.66	0.0003
288.86	0.0009	288.86	0.0008	288.73	0.0012	288.73	0.0012

Table S3: nit8 C1s excitation energies (in eV) and oscillator strengths at the TDDFT-BLYP-SRC1/6-311(2+)G* level.

C1		C2		C3		C4		C5	
286.67	0.0381	288.42	0.0000	288.36	0.0000	288.11	0.0001	287.71	0.0077
288.94	0.0303	289.41	0.0002	289.11	0.0225	288.22	0.0080	287.90	0.0002
290.88	0.0001	289.46	0.0001	289.45	0.0005	288.52	0.0008	288.21	0.0019
290.99	0.0012	289.52	0.0358	289.46	0.0023	288.66	0.0022	288.36	0.0175
291.09	0.0003	289.84	0.0029	289.57	0.0194	288.79	0.0001	288.88	0.0003
291.72	0.0005	289.95	0.0001	289.75	0.0011	288.97	0.0069	288.97	0.0014
291.77	0.0001	289.99	0.0017	290.02	0.0005	289.26	0.0008	289.02	0.0007
291.86	0.0001	290.08	0.0001	290.06	0.0004	289.29	0.0002	289.07	0.0000
291.94	0.0001	290.28	0.0020	290.07	0.0022	289.44	0.0002	289.25	0.0005
291.97	0.0002	290.29	0.0014	290.19	0.0012	289.48	0.0001	289.26	0.0014
292.02	0.0000	290.30	0.0039	290.19	0.0011	289.52	0.0000	289.34	0.0007
292.27	0.0001	290.42	0.0001	290.25	0.0003	289.70	0.0028	289.35	0.0019
292.33	0.0000	290.52	0.0032	290.45	0.0047	289.84	0.0001	289.54	0.0022
292.40	0.0008	290.52	0.0020	290.55	0.0009	289.91	0.0017	289.57	0.0004
292.46	0.0008	290.59	0.0000	290.58	0.0000	289.94	0.0011	289.71	0.0048
292.47	0.0000	290.69	0.0029	290.64	0.0003	289.96	0.0027	289.74	0.0002
292.49	0.0001	290.73	0.0001	290.67	0.0001	289.98	0.0000	289.77	0.0001
292.50	0.0000	290.75	0.0002	290.67	0.0012	290.00	0.0000	289.79	0.0002
292.55	0.0000	290.79	0.0000	290.68	0.0005	290.04	0.0022	289.81	0.0000
292.55	0.0010	290.81	0.0023	290.77	0.0000	290.05	0.0000	289.84	0.0000

C6		C7		C8		C9	
287.03	0.0009	287.05	0.0005	286.79	0.0008	286.66	0.0004
287.36	0.0048	287.33	0.0053	287.36	0.0041	287.31	0.0052
287.75	0.0011	287.70	0.0009	287.60	0.0005	287.48	0.0002
287.98	0.0130	287.99	0.0117	287.90	0.0024	287.61	0.0020
288.08	0.0027	288.06	0.0033	288.06	0.0012	287.81	0.0011
288.19	0.0008	288.21	0.0005	288.07	0.0001	287.87	0.0032
288.37	0.0098	288.32	0.0058	288.16	0.0084	288.06	0.0001
288.42	0.0006	288.35	0.0003	288.19	0.0012	288.07	0.0003
288.63	0.0003	288.54	0.0079	288.30	0.0003	288.10	0.0002
288.68	0.0040	288.56	0.0005	288.31	0.0020	288.28	0.0006
288.79	0.0008	288.75	0.0003	288.49	0.0002	288.32	0.0000
288.79	0.0001	288.78	0.0001	288.52	0.0080	288.34	0.0077
288.92	0.0002	288.85	0.0031	288.67	0.0071	288.48	0.0048
288.94	0.0023	288.86	0.0002	288.72	0.0005	288.50	0.0032
289.04	0.0004	288.98	0.0014	288.75	0.0001	288.56	0.0001
289.06	0.0015	289.03	0.0012	288.83	0.0002	288.57	0.0013
289.07	0.0000	289.04	0.0000	288.85	0.0005	288.58	0.0001
289.13	0.0001	289.06	0.0011	288.86	0.0000	288.63	0.0001
289.15	0.0012	289.10	0.0001	288.91	0.0007	288.73	0.0001
289.17	0.0001	289.11	0.0002	288.94	0.0000	288.73	0.0002

Table S4: nit8 C1s excitation energies (in eV) and oscillator strengths at the TDDFT-BLYP-SRC2/6-311(2+)G* level.

C1		C2		C3		C4		C5	
287.13	0.0139	287.62	0.0000	287.56	0.0000	287.06	0.0000	286.79	0.0000
288.37	0.0582	289.14	0.0000	288.61	0.0050	287.93	0.0013	287.81	0.0029
289.73	0.0001	289.17	0.0000	288.85	0.0032	287.99	0.0003	287.99	0.0010
290.99	0.0007	289.35	0.0004	289.31	0.0002	288.48	0.0015	288.07	0.0005
291.04	0.0005	289.40	0.0000	289.35	0.0001	288.55	0.0006	288.17	0.0021
291.66	0.0004	289.70	0.0270	289.65	0.0266	288.92	0.0064	288.58	0.0110
291.69	0.0002	289.85	0.0031	289.87	0.0001	289.12	0.0011	288.84	0.0005
291.88	0.0001	289.91	0.0002	289.91	0.0000	289.19	0.0004	288.87	0.0013
291.89	0.0000	290.09	0.0008	290.04	0.0008	289.30	0.0008	289.00	0.0013
291.98	0.0001	290.14	0.0001	290.09	0.0001	289.42	0.0000	289.12	0.0006
291.99	0.0000	290.23	0.0001	290.14	0.0002	289.45	0.0000	289.16	0.0002
292.27	0.0001	290.27	0.0038	290.20	0.0035	289.68	0.0020	289.30	0.0027
292.29	0.0000	290.48	0.0009	290.45	0.0009	289.75	0.0002	289.43	0.0009
292.42	0.0006	290.52	0.0048	290.50	0.0000	289.88	0.0009	289.47	0.0026
292.45	0.0001	290.53	0.0001	290.55	0.0024	289.90	0.0023	289.61	0.0013
292.47	0.0011	290.67	0.0003	290.62	0.0000	289.91	0.0014	289.62	0.0025
292.50	0.0000	290.69	0.0016	290.62	0.0005	289.92	0.0001	289.69	0.0001
292.50	0.0001	290.73	0.0003	290.65	0.0002	289.95	0.0001	289.69	0.0000
292.52	0.0000	290.75	0.0005	290.67	0.0013	289.97	0.0001	289.71	0.0000
292.57	0.0007	290.75	0.0001	290.69	0.0001	290.01	0.0014	289.71	0.0005

C6		C7		C8		C9	
285.92	0.0008	285.91	0.0005	285.67	0.0008	285.52	0.0004
287.29	0.0009	287.33	0.0010	287.04	0.0001	286.84	0.0008
287.38	0.0008	287.38	0.0003	287.05	0.0003	286.86	0.0004
287.58	0.0009	287.47	0.0007	287.31	0.0006	287.21	0.0000
287.63	0.0005	287.54	0.0008	287.36	0.0006	287.21	0.0001
287.86	0.0015	287.85	0.0009	287.82	0.0012	287.62	0.0020
288.01	0.0021	288.00	0.0013	287.94	0.0003	287.72	0.0006
288.19	0.0058	288.11	0.0061	287.97	0.0005	287.81	0.0003
288.33	0.0009	288.26	0.0009	288.05	0.0018	287.89	0.0010
288.35	0.0023	288.30	0.0021	288.11	0.0013	287.93	0.0004
288.43	0.0006	288.38	0.0005	288.16	0.0004	287.97	0.0002
288.60	0.0043	288.55	0.0044	288.44	0.0047	288.31	0.0035
288.72	0.0006	288.66	0.0005	288.51	0.0005	288.33	0.0004
288.77	0.0031	288.72	0.0038	288.54	0.0009	288.33	0.0001
288.86	0.0006	288.83	0.0001	288.61	0.0043	288.38	0.0013
288.88	0.0001	288.84	0.0001	288.63	0.0005	288.42	0.0005
288.92	0.0015	288.88	0.0005	288.68	0.0002	288.45	0.0002
288.93	0.0004	288.88	0.0012	288.71	0.0008	288.48	0.0027
288.96	0.0002	288.91	0.0001	288.72	0.0001	288.53	0.0001
289.00	0.0010	288.93	0.0007	288.73	0.0009	288.53	0.0005

Table S5: nit9 C1s excitation energies (in eV) and oscillator strengths at the TDDFT-BLYP-SRC1/6-311(2+)G* level.

C1		C2		C3		C4		C5	
286.66	0.0403	288.36	0.0001	288.21	0.0011	284.62	0.0126	285.02	0.0326
288.72	0.0130	288.37	0.0000	288.26	0.0001	285.83	0.0102	286.09	0.0238
291.00	0.0000	288.61	0.0000	288.43	0.0000	288.16	0.0001	288.13	0.0001
291.15	0.0013	289.54	0.0186	289.35	0.0274	288.29	0.0057	288.64	0.0004
291.24	0.0002	289.68	0.0000	289.59	0.0000	288.63	0.0015	288.71	0.0001
291.33	0.0074	289.73	0.0176	289.63	0.0100	289.28	0.0012	289.21	0.0067
291.89	0.0005	290.07	0.0023	290.04	0.0019	289.35	0.0001	289.32	0.0013
291.92	0.0000	290.17	0.0001	290.12	0.0000	289.41	0.0014	289.34	0.0001
292.07	0.0008	290.34	0.0041	290.22	0.0028	289.57	0.0003	289.48	0.0002
292.13	0.0001	290.44	0.0001	290.26	0.0001	289.58	0.0007	289.54	0.0000
292.18	0.0001	290.46	0.0035	290.31	0.0018	289.66	0.0002	289.60	0.0005
292.21	0.0000	290.51	0.0001	290.39	0.0000	289.80	0.0014	289.62	0.0000
292.43	0.0003	290.72	0.0009	290.47	0.0050	289.93	0.0002	289.86	0.0002
292.48	0.0000	290.76	0.0043	290.63	0.0033	290.00	0.0001	289.90	0.0000
292.56	0.0014	290.79	0.0000	290.67	0.0001	290.04	0.0002	290.00	0.0002
292.57	0.0003	290.86	0.0025	290.72	0.0005	290.08	0.0000	290.02	0.0000
292.62	0.0000	290.92	0.0001	290.75	0.0001	290.09	0.0000	290.04	0.0008
292.64	0.0005	290.93	0.0000	290.77	0.0000	290.10	0.0006	290.04	0.0003
292.67	0.0001	290.95	0.0011	290.82	0.0003	290.16	0.0003	290.08	0.0004
292.71	0.0000	291.01	0.0006	290.86	0.0000	290.17	0.0000	290.12	0.0001

C6		C7		C8		C9	
286.77	0.0001	286.75	0.0000	286.55	0.0010	286.38	0.0014
286.88	0.0029	286.85	0.0030	286.60	0.0003	286.46	0.0006
287.26	0.0001	287.22	0.0001	286.79	0.0008	286.63	0.0010
287.45	0.0062	287.50	0.0057	287.41	0.0044	287.44	0.0034
287.86	0.0011	287.88	0.0008	287.65	0.0004	287.58	0.0002
288.12	0.0128	288.16	0.0025	287.88	0.0016	287.74	0.0018
288.23	0.0040	288.21	0.0135	288.15	0.0018	288.03	0.0009
288.37	0.0004	288.31	0.0007	288.18	0.0055	288.07	0.0048
288.57	0.0110	288.49	0.0113	288.23	0.0001	288.17	0.0003
288.64	0.0006	288.68	0.0005	288.25	0.0054	288.20	0.0044
288.79	0.0032	288.72	0.0002	288.47	0.0002	288.31	0.0001
288.79	0.0002	288.75	0.0036	288.54	0.0102	288.40	0.0048
289.01	0.0030	288.94	0.0028	288.60	0.0033	288.53	0.0071
289.03	0.0002	289.00	0.0002	288.72	0.0011	288.57	0.0010
289.15	0.0021	289.11	0.0001	288.75	0.0001	288.61	0.0001
289.18	0.0001	289.14	0.0014	288.80	0.0002	288.68	0.0002
289.20	0.0002	289.14	0.0002	288.82	0.0008	288.69	0.0005
289.21	0.0001	289.16	0.0000	288.83	0.0001	288.70	0.0000
289.22	0.0012	289.23	0.0018	288.92	0.0001	288.77	0.0001
289.27	0.0004	289.25	0.0001	288.93	0.0007	288.82	0.0009

Table S6: nit9 C1s excitation energies (in eV) and oscillator strengths at the TDDFT-BLYP-SRC2/6-311(2+)G* level.

C1		C2		C3		C4		C5	
287.08	0.0213	287.61	0.0000	287.47	0.0000	285.07	0.0000	284.98	0.0135
288.17	0.0292	287.63	0.0000	287.48	0.0005	285.63	0.0002	285.57	0.0517
289.82	0.0000	287.81	0.0000	287.63	0.0000	287.04	0.0001	287.01	0.0001
290.86	0.0090	289.54	0.0035	289.38	0.0070	288.50	0.0007	288.44	0.0006
291.16	0.0008	289.60	0.0000	289.47	0.0000	288.57	0.0016	288.53	0.0010
291.21	0.0005	289.85	0.0251	289.69	0.0230	288.94	0.0024	288.99	0.0070
291.62	0.0073	290.04	0.0013	289.93	0.0018	289.18	0.0002	289.15	0.0008
291.83	0.0003	290.11	0.0001	290.00	0.0001	289.21	0.0003	289.19	0.0010
291.87	0.0007	290.40	0.0021	290.21	0.0030	289.39	0.0012	289.38	0.0005
292.07	0.0006	290.41	0.0002	290.23	0.0003	289.41	0.0006	289.39	0.0025
292.12	0.0001	290.47	0.0036	290.26	0.0029	289.47	0.0007	289.45	0.0010
292.21	0.0000	290.48	0.0002	290.33	0.0006	289.55	0.0003	289.52	0.0003
292.22	0.0001	290.62	0.0004	290.35	0.0000	289.58	0.0000	289.56	0.0011
292.43	0.0002	290.68	0.0001	290.43	0.0005	289.78	0.0006	289.74	0.0004
292.46	0.0000	290.72	0.0012	290.59	0.0014	289.82	0.0003	289.79	0.0004
292.54	0.0013	290.77	0.0001	290.62	0.0002	289.94	0.0003	289.91	0.0001
292.60	0.0001	290.88	0.0024	290.73	0.0002	289.97	0.0000	289.94	0.0000
292.67	0.0003	290.89	0.0002	290.74	0.0011	290.03	0.0002	290.00	0.0005
292.70	0.0001	290.94	0.0017	290.81	0.0009	290.06	0.0002	290.03	0.0003
292.71	0.0001	291.00	0.0001	290.84	0.0001	290.07	0.0001	290.04	0.0002

C6		C7		C8		C9	
285.76	0.0002	285.72	0.0002	285.53	0.0002	285.38	0.0004
285.88	0.0023	285.84	0.0022	285.53	0.0003	285.40	0.0002
286.12	0.0001	286.08	0.0001	285.65	0.0009	285.49	0.0014
287.52	0.0021	287.56	0.0015	287.34	0.0007	287.27	0.0002
287.68	0.0014	287.69	0.0008	287.38	0.0004	287.28	0.0003
288.02	0.0008	287.95	0.0013	287.79	0.0015	287.66	0.0013
288.15	0.0014	288.10	0.0018	287.93	0.0003	287.78	0.0005
288.28	0.0066	288.32	0.0062	287.96	0.0001	287.89	0.0006
288.48	0.0011	288.48	0.0020	288.04	0.0012	287.99	0.0009
288.56	0.0022	288.49	0.0010	288.22	0.0022	288.08	0.0015
288.61	0.0004	288.54	0.0007	288.27	0.0003	288.12	0.0004
288.73	0.0050	288.65	0.0033	288.34	0.0026	288.16	0.0007
288.83	0.0010	288.76	0.0017	288.42	0.0002	288.25	0.0002
288.84	0.0004	288.77	0.0026	288.49	0.0022	288.39	0.0051
288.89	0.0004	288.87	0.0004	288.52	0.0029	288.41	0.0009
288.91	0.0025	288.89	0.0015	288.54	0.0002	288.43	0.0001
289.02	0.0004	288.96	0.0004	288.61	0.0035	288.51	0.0005
289.04	0.0022	289.00	0.0021	288.62	0.0006	288.51	0.0027
289.12	0.0009	289.08	0.0003	288.73	0.0003	288.60	0.0003
289.13	0.0009	289.09	0.0014	288.76	0.0020	288.63	0.0024

Table S7: tempo N1s excitation energies (in eV) and oscillator strengths at the TDDFT-BLYP-SRC1/6-311(2+)G* and TDDFT-BLYP-SRC2/6-311(2+)G* levels.

N1	src1	N1	src2
400.35	0.0147	399.89	0.0169
404.96	0.0000	404.50	0.0000
405.19	0.0036	404.80	0.0018
405.34	0.0000	404.91	0.0000
405.40	0.0000	404.99	0.0000
405.47	0.0000	405.06	0.0000
405.55	0.0087	405.22	0.0041
405.61	0.0020	405.22	0.0013
405.75	0.0003	405.35	0.0006
405.80	0.0005	405.37	0.0000
405.85	0.0059	405.49	0.0034
405.92	0.0000	405.53	0.0000
405.96	0.0000	405.57	0.0000
406.00	0.0000	405.61	0.0000
406.05	0.0000	405.67	0.0000
406.21	0.0000	405.77	0.0000
406.21	0.0048	405.87	0.0026
406.31	0.0003	405.95	0.0000
406.32	0.0014	405.95	0.0001
406.33	0.0024	405.96	0.0001
406.38	0.0000	405.97	0.0004
406.39	0.0000	406.01	0.0003
406.43	0.0047	406.05	0.0000
406.46	0.0001	406.06	0.0000
406.47	0.0000	406.09	0.0024
406.52	0.0001	406.13	0.0007
406.54	0.0002	406.15	0.0000
406.55	0.0113	406.18	0.0006
406.58	0.0010	406.21	0.0003
406.58	0.0000	406.22	0.0000

Table S8: nit8 N1s excitation energies (in eV) and oscillator strengths at the TDDFT-BLYP-SRC1/6-311(2+)G* and TDDFT-BLYP-SRC2/6-311(2+)G* levels.

N1	src1	N2	src1	N1	src2	N2	src2
400.36	0.0155	402.42	0.0140	399.93	0.0177	401.72	0.0060
404.78	0.0000	402.49	0.0056	404.04	0.0000	402.00	0.0019
405.13	0.0015	403.24	0.0058	404.32	0.0000	402.18	0.0106
405.22	0.0000	403.32	0.0052	404.41	0.0011	402.36	0.0023
405.36	0.0000	403.36	0.0198	404.69	0.0003	402.93	0.0038
405.49	0.0035	403.70	0.0002	404.85	0.0000	403.39	0.0150
405.52	0.0004	404.34	0.0017	405.06	0.0000	403.83	0.0014
405.64	0.0001	404.37	0.0006	405.12	0.0000	403.85	0.0019
405.72	0.0015	404.46	0.0010	405.24	0.0008	404.06	0.0008
405.75	0.0024	404.54	0.0006	405.39	0.0008	404.07	0.0010
405.87	0.0001	404.68	0.0003	405.45	0.0000	404.18	0.0010
405.89	0.0055	404.76	0.0007	405.48	0.0006	404.29	0.0007
405.99	0.0000	404.96	0.0003	405.58	0.0001	404.41	0.0011
406.01	0.0000	404.99	0.0010	405.64	0.0000	404.55	0.0010
406.07	0.0000	405.10	0.0006	405.65	0.0001	404.65	0.0004
406.10	0.0000	405.15	0.0002	405.72	0.0002	404.67	0.0005
406.16	0.0044	405.17	0.0002	405.75	0.0014	404.72	0.0002
406.21	0.0003	405.20	0.0001	405.81	0.0004	404.73	0.0002
406.23	0.0040	405.21	0.0001	405.84	0.0015	404.75	0.0001
406.34	0.0079	405.24	0.0000	405.96	0.0000	404.76	0.0001
406.37	0.0045	405.28	0.0003	405.99	0.0001	404.81	0.0001
406.39	0.0001	405.28	0.0000	406.01	0.0006	404.83	0.0002
406.40	0.0013	405.32	0.0001	406.01	0.0029	404.86	0.0000
406.42	0.0001	405.33	0.0009	406.07	0.0031	404.91	0.0010
406.47	0.0060	405.49	0.0004	406.08	0.0044	405.01	0.0002
				406.14	0.0013	405.02	0.0002
				406.15	0.0099	405.04	0.0004
				406.18	0.0057	405.05	0.0002

Table S9: nit9 N1s excitation energies (in eV) and oscillator strengths at the TDDFT-BLYP-SRC1/6-311(2+)G* and TDDFT-BLYP-SRC2/6-311(2+)G* levels.

N1	src1	N2	src1	N1	src2	N2	src2
400.36	0.0157	401.70	0.0086	399.93	0.0180	400.79	0.0033
403.83	0.0000	402.22	0.0036	402.61	0.0000	401.03	0.0069
404.20	0.0001	402.40	0.0064	403.00	0.0001	401.90	0.0000
404.92	0.0000	403.21	0.0048	404.44	0.0000	402.30	0.0029
405.23	0.0022	403.28	0.0195	404.80	0.0008	402.87	0.0043
405.40	0.0000	403.59	0.0000	404.96	0.0000	403.31	0.0143
405.59	0.0000	404.29	0.0030	405.19	0.0000	403.76	0.0014
405.70	0.0000	404.30	0.0007	405.32	0.0001	403.80	0.0035
405.73	0.0018	404.43	0.0020	405.33	0.0015	403.89	0.0029
405.77	0.0048	404.59	0.0003	405.41	0.0014	404.02	0.0028
405.99	0.0001	404.65	0.0004	405.48	0.0000	404.13	0.0001
406.06	0.0028	404.71	0.0011	405.60	0.0002	404.14	0.0004
406.08	0.0015	404.88	0.0020	405.69	0.0012	404.24	0.0010
406.11	0.0000	404.89	0.0004	405.71	0.0008	404.31	0.0003
406.13	0.0075	404.98	0.0004	405.76	0.0029	404.39	0.0008
406.18	0.0002	405.07	0.0005	405.82	0.0001	404.50	0.0011
406.24	0.0002	405.07	0.0003	405.85	0.0018	404.60	0.0004
406.26	0.0150	405.11	0.0001	405.88	0.0005	404.65	0.0006
406.31	0.0001	405.11	0.0002	405.92	0.0000	404.70	0.0001
406.40	0.0052	405.16	0.0001	405.93	0.0001	404.71	0.0004
406.46	0.0029	405.20	0.0000	406.03	0.0007	404.73	0.0003
406.51	0.0001	405.22	0.0001	406.11	0.0001	404.74	0.0001
406.53	0.002	405.24	0.0001	406.16	0.0076	404.78	0.0001
406.55	0.0010	405.26	0.0013	406.17	0.0019	404.81	0.0001
406.56	0.0001	405.34	0.0008	406.19	0.0033	404.83	0.0000
		405.45	0.0003	406.22	0.0014	404.87	0.0016
				406.24	0.0001	404.97	0.0002
				406.26	0.0000	405.00	0.0001
				406.31	0.0003	405.08	0.0002
				406.34	0.0000	405.09	0.0001

Table S10: tempo O1s excitation energies (in eV) and oscillator strengths at the TDDFT-BLYP-SRC1/6-311(2+)G* and TDDFT-BLYP-SRC2/6-311(2+)G* levels.

O1	src1	O1	src2
529.67	0.0178	529.16	0.0197
535.61	0.0000	534.85	0.0000
535.85	0.0224	535.25	0.0000
535.97	0.0000	535.27	0.0059
536.04	0.0000	535.32	0.0000
536.04	0.0005	535.35	0.0000
536.13	0.0020	535.55	0.0097
536.43	0.0000	535.69	0.0001
536.48	0.0000	535.74	0.0000
536.51	0.0000	535.81	0.0000
536.53	0.0001	535.83	0.0000
536.55	0.0000	535.87	0.0000
536.58	0.0000	535.92	0.0000
536.61	0.0000	535.96	0.0000
536.71	0.0067	536.06	0.0047
536.81	0.0000	536.08	0.0001
536.94	0.0013	536.26	0.0001
536.98	0.0000	536.27	0.0045
536.99	0.0000	536.27	0.0000
537.00	0.0002	536.32	0.0001
537.04	0.0000	536.35	0.0004
537.05	0.0000	536.36	0.0001
537.06	0.0001	536.38	0.0000
537.07	0.0000	536.40	0.0002
537.09	0.0006	536.43	0.0001
537.12	0.0001	536.46	0.0000
537.12	0.0000	536.46	0.0016
537.17	0.0000	536.51	0.0001
537.20	0.0000	536.52	0.0000
537.22	0.0000	536.56	0.0000

Table S11: nit8 O1s excitation energies (in eV) and oscillator strengths at the TDDFT-BLYP-SRC1/6-311(2+)G* and TDDFT-BLYP-SRC2/6-311(2+)G* levels.

O1	src1	O2	src1	O1	src2	O2	src2
529.99	0.0176	531.78	0.0190	529.44	0.0196	531.32	0.0095
535.58	0.0000	533.31	0.0142	534.53	0.0000	532.21	0.0228
535.81	0.0214	534.83	0.0000	534.79	0.0000	533.03	0.0001
536.01	0.0007	534.92	0.0009	534.91	0.0053	534.28	0.0005
536.10	0.0013	535.02	0.0004	535.20	0.0023	534.33	0.0006
536.13	0.0000	535.61	0.0004	535.29	0.0000	534.93	0.0003
536.25	0.0001	535.67	0.0001	535.51	0.0000	534.96	0.0002
536.45	0.0001	535.70	0.0003	535.56	0.0001	535.12	0.0001
536.59	0.0024	535.78	0.0001	535.71	0.0039	535.15	0.0002
536.60	0.0001	535.83	0.0002	535.86	0.0041	535.22	0.0001
536.61	0.0002	535.88	0.0001	535.89	0.0003	535.24	0.0001
536.73	0.0000	536.15	0.0006	536.03	0.0001	535.52	0.0004
536.73	0.0000	536.21	0.0000	536.03	0.0000	535.55	0.0001
536.77	0.0015	536.28	0.0001	536.06	0.0000	535.67	0.0001
536.80	0.0000	536.33	0.0001	536.10	0.0000	535.71	0.0000
536.82	0.0001	536.33	0.0000	536.15	0.0000	535.74	0.0000
536.96	0.0000	536.33	0.0000	536.23	0.0035	535.74	0.0001
537.04	0.0009	536.36	0.0000	536.25	0.0033	535.75	0.0000
537.13	0.0000	536.39	0.0000	536.40	0.0001	535.76	0.0001
537.14	0.0001	536.44	0.0000	536.41	0.0010	535.84	0.0001
537.16	0.0024	536.46	0.0003	536.42	0.0013	535.86	0.0000
537.19	0.0004	536.47	0.0000	536.50	0.0000	535.86	0.0001
537.20	0.0000	536.53	0.0000	536.52	0.0003	535.89	0.0001
537.22	0.0009	536.67	0.0001	536.55	0.0010	536.03	0.0001
537.27	0.0001	536.70	0.0000	536.58	0.0000	536.05	0.0000
				536.58	0.0006	536.08	0.0001
				536.62	0.0002	536.10	0.0000
				536.66	0.0000	536.16	0.0000
				536.68	0.0000	536.17	0.0000
				536.72	0.0000	536.23	0.0004
						536.26	0.0001

Table S12: nit9 O1s excitation energies (in eV) and oscillator strengths at the TDDFT-BLYP-SRC1/6-311(2+)G* and TDDFT-BLYP-SRC2/6-311(2+)G* levels.

O1	src1	O2	src1	O1	src2	O2	src2
529.95	0.0180	531.15	0.0199	529.41	0.0200	530.62	0.0083
534.78	0.0000	532.75	0.0096	533.15	0.0000	531.38	0.0199
535.28	0.0003	534.97	0.0000	533.63	0.0001	533.13	0.0000
535.72	0.0000	535.12	0.0009	534.92	0.0000	534.47	0.0005
535.97	0.0232	535.22	0.0004	535.35	0.0053	534.53	0.0006
536.14	0.0011	535.81	0.0009	535.40	0.0002	534.79	0.0028
536.23	0.0008	535.86	0.0001	535.59	0.0083	535.02	0.0031
536.33	0.0002	535.97	0.0006	535.67	0.0032	535.14	0.0003
536.44	0.0000	536.00	0.0019	535.77	0.0000	535.17	0.0007
536.70	0.0026	536.05	0.0001	535.96	0.0004	535.37	0.0001
536.72	0.0000	536.13	0.0001	535.98	0.0026	535.40	0.0001
536.83	0.0000	536.17	0.0008	536.05	0.0001	535.49	0.0000
536.84	0.0000	536.36	0.0006	536.16	0.0000	535.51	0.0000
536.89	0.0000	536.41	0.0000	536.23	0.0000	535.71	0.0005
536.90	0.0045	536.48	0.0000	536.25	0.0003	535.75	0.0001
536.94	0.0001	536.51	0.0000	536.27	0.0043	535.84	0.0001
536.96	0.0000	536.53	0.0000	536.32	0.0000	535.87	0.0000
537.06	0.0000	536.56	0.0002	536.36	0.0000	535.95	0.0002
537.19	0.0005	536.57	0.0003	536.38	0.0001	535.98	0.0000
537.24	0.0000	536.62	0.0000	536.45	0.0006	535.98	0.0001
537.29	0.0001	536.66	0.0004	536.53	0.0001	536.00	0.0001
537.30	0.0003	536.67	0.0000	536.57	0.0010	536.02	0.0001
537.34	0.0004	536.69	0.0003	536.61	0.0001	536.05	0.0001
537.35	0.0001	536.73	0.0000	536.67	0.0006	536.07	0.0001
537.38	0.0002	536.94	0.0001	536.68	0.0002	536.09	0.0000
537.38	0.0000			536.69	0.0000	536.26	0.0001
537.41	0.0000			536.71	0.0007	536.28	0.0000
537.43	0.0000			536.77	0.0000	536.34	0.0001
537.44	0.0002			536.79	0.0000	536.35	0.0000
537.46	0.0000			536.80	0.0001	536.37	0.0002

Table S13: tempo excitation energies (in eV) and total spin expectation values at the ΔB3LYP/cc-pwCVTZ/mcp-dzp/cc-pVDZ(H) level.

	O1	**N1**	**C1**	**C2**	**C3**	**C4**
E	528.99	399.34	286.89	286.89	286.81	286.81
$\langle S^2 \rangle$	0.757	0.761	0.766	0.766	0.876	0.876
	C5	**C6**	**C7**	**C8**	**C9**	
E	287.20	286.44	286.44	286.33	286.33	
$\langle S^2 \rangle$	0.952	0.775	0.775	0.761	0.761	

Table S14: nit8 excitation energies (in eV) and total spin expectation values at the ΔB3LYP/cc-pwCVTZ/mcp-dzp/cc-pVDZ(H) level.

	O1	**O2**	**N1**	**N2**	**C1**	**C2**	**C3**
E	529.27	531.22	399.44	401.63	287.45	287.19	287.09
$\langle S^2 \rangle$	0.757	1.762	0.760	1.756	1.760	0.763	0.764
	C4	**C5**	**C6**	**C7**	**C8**	**C9**	
E	287.21	287.14	286.65	286.75	286.43	286.41	
$\langle S^2 \rangle$	1.085	1.078	0.805	0.802	0.767	0.762	

Table S15: nit9 excitation energies (in eV) and total spin expectation values at the ΔB3LYP/cc-pwCVTZ/mcp-dzp/cc-pVDZ(H) level.

	O1	**O2**	**N1**	**N2**	**C1**	**C2**	**C3**
E	529.27	530.52	399.47	400.79	287.17	287.15	287.05
$\langle S^2 \rangle$	0.757	1.773	0.760	1.768	1.768	1.052	1.023
	C4	**C5**	**C6**	**C7**	**C8**	**C9**	
E	284.38	284.59	286.56	286.49	286.44	286.25	
$\langle S^2 \rangle$	1.766	1.765	1.080	1.028	1.069	1.039	