Supplementary Material for "Fractional-Electron and Transition-Potential Methods for Core-to-Valence Excitation Energies Using Density Functional Theory"

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May 24, 2023

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Table S1: Excitation energies (in eV) for 37 K-edge (1s → LUMO) transitions computed using various methods with the SRC1-r1 functional, including relativistic corrections.

Molecule	Atom	Expt.	ΔSCF	STM	GSTM	TPM	GSTM	FCHM	XCHM	IP-TPM@1/2	IP-TPM@1/3
C_2H_4	C	284.7	286.9	287.1	288.0	288.5	289.9	283.3	285.9	288.0	286.4
HCHO	C	285.6	287.0	287.7	287.0	290.2	289.6	284.7	279.2	289.6	287.7
C_2H_2	C	285.9	287.9	288.1	289.2	289.6	291.3	284.4	287.4	289.1	287.4
C_2N_2	C	286.3	288.1	288.2	289.1	290.1	290.7	285.4	287.8	289.6	288.3
HCN	C	286.4	287.5	288.2	287.6	290.6	290.0	285.5	280.2	290.1	288.2
acetone	C (CO)	286.4	287.5	288.3	287.6	290.7	290.2	284.9	279.7	290.1	288.5
C_2H_6	C	286.9	288.8	289.2	289.7	291.0	290.9	287.0	290.1	289.8	288.9
CO	C	287.4	288.0	288.7	288.1	291.8	291.3	286.9	280.1	291.3	289.1
CH_4	C	288.0	288.2	288.7	288.3	290.2	289.7	287.1	284.3	289.7	288.7
MeOH	C	288.0	289.7	290.4	289.8	291.7	291.4	288.2	285.5	291.2	289.7
HCOOH	C	288.1	289.1	289.8	289.2	292.5	291.9	287.0	281.3	291.9	290.0
HCOF	C	288.2	289.3	290.0	289.4	292.8	292.3	287.3	281.3	292.2	290.3
CO_2	C	290.8	291.4	292.1	291.2	295.2	294.3	290.0	283.5	294.6	292.5
CF_2O	C	290.9	291.7	292.4	291.8	295.5	297.0	289.9	283.3	294.9	294.0
MAE	C(1s)		1.26	1.81	1.59	4.06	4.06	0.90	4.92	3.46	1.87
C_2N_2	N	398.9	400.0	400.7	402.1	403.8	403.8	395.6	400.1	401.9	400.4
HCN	N	399.7	400.7	401.5	400.8	403.8	403.2	396.8	391.9	403.2	401.3
Imidazole	N	399.9									
NH_3	N	400.8	402.0	402.8	402.2	404.3	403.8	399.6	396.4	403.7	402.5
N_2	N	400.9	401.7	403.3	404.6	405.4	407.8	398.6	392.3	404.8	402.6
N_2O	N	401.0									
Glycine	N	401.2	402.6	403.5	402.7	404.7	404.0	399.7	397.0	404.1	403.0
Pyrrole	N	402.3	403.5	404.5	403.9	405.4	404.7	399.5	397.0	404.8	403.7
Imidazole	NH	402.3	401.0	404.1	403.5	405.6	404.9	399.6	402.9	405.0	403.7
N_2O	N (center)	404.6	405.4	402.7	408.3	408.9	407.4	401.9	396.1	408.3	406.7
MAE	N(1s)		1.10	2.03	2.18	3.89	3.61	2.42	5.08	3.14	1.66
HCHO	O	530.8	531.8	532.5	532.0	534.7	534.1	527.0	522.8	534.0	532.3
acetone	O	531.4	532.1	532.7	532.3	534.8	534.3	527.3	523.5	534.1	532.7
HCOF	O	532.1	532.8	533.5	533.0	535.7	535.2	528.2	524.1	535.0	533.3
HCOOH	O	532.2									
CF_2O	O	532.7	533.8	534.4	534.0	536.7	536.2	529.3	525.1	536.1	534.3
H_2O	O	534.0	535.2	536.0	535.4	537.8	537.3	532.2	528.5	537.2	535.8
MeOH	O	534.1	535.3	536.2	535.5	537.6	537.0	531.6	528.7	537.0	535.7
CO	O	534.2	534.9	535.6	535.0	538.0	537.4	530.5	525.8	537.4	535.4
N_2O	O	534.6	535.7	536.3	535.8	538.0	537.6	530.7	527.5	537.4	535.8
Furan	O	535.2	536.1	536.7	536.3	538.1	537.6	531.3	528.8	537.5	536.3
HCOOH	OH	535.4	536.5	533.4	536.7	538.4	538.9	532.1	529.7	537.8	535.5
CO_2	O	535.4	536.3	536.9	538.2	539.0	540.6	541.0	536.0	538.3	536.6
MAE	O(1s)		0.97	1.67	1.29	3.54	3.30	3.62	6.43	2.90	1.24
F_2	F	682.2	682.8	685.0	685.7	687.4	689.9	688.5	670.4	686.7	684.0
HF	F	687.4	688.6	689.3	688.8	691.5	691.0	685.9	681.8	690.9	689.2
HCOF	F	687.7	688.7	689.4	688.9	690.7	690.2	684.5	682.1	690.0	688.6
CF_2O	F	689.2	690.3	690.9	691.2	692.8	692.4	686.2	689.0	691.6	690.2
MAE	F(1s)		0.97	2.00	2.04	3.99	4.26	3.52	5.79	3.17	1.37
MAE	all		1.11	1.84	1.68	3.86	3.76	2.32	5.50	3.19	1.58

Table S2: Excitation energies (in eV) for 20 higher-lying K-edge transitions computed using various methods with the SRC1-r1 functional, including relativistic corrections.

Molecule	Atom	Expt.	ΔSCF	XCHM	XTPM	XGTPM	IP-TPM@1/2	IP-TPM@1/3
NH_3	N	402.33	403.75	397.85	405.00	404.22	405.83	404.61
NH_3	N	402.86	403.80	398.02	405.00	404.22	405.83	404.61
NH_3	N	403.57	405.08	400.22	406.02	405.25	406.93	405.95
HCHO (formaldehyde)	C	290.18	291.72	287.57	291.24	290.52	293.30	292.20
HCHO (formaldehyde)	C	291.25	293.30	289.61	292.50	291.75	294.61	293.50
HCHO (formaldehyde)	C	291.73	292.73	288.06	292.60	291.87	294.77	293.79
HCHO (formaldehyde)	O	535.43	536.55	530.88	536.02	535.00	537.85	536.91
HCHO (formaldehyde)	O	536.34	537.45	531.18	537.20	536.15	539.02	537.99
CO	C	292.37	294.40	292.34	292.66	291.93	296.03	295.07
CO	C	293.33	295.63	294.27	293.70	292.97	297.26	296.38
CO	C	293.49	295.45	293.93	293.76	293.04	297.33	296.49
CO	O	538.91	539.97	534.81	539.04	537.97	541.57	540.63
CO	O	539.91	541.21	536.70	540.13	539.05	542.84	542.00
N_2	N	406.10	408.16	403.89	409.47	409.00	412.15	411.11
N_2	N	407.00	409.11	405.72	409.94	409.47	412.77	411.58
N_2O	NC	407.60	410.61	403.76	409.34	410.82	412.49	411.05
C_2H_4 (ethylene)	C	287.24	288.74	284.55	290.15	289.84	290.33	289.41
C_2H_4 (ethylene)	C	287.88	289.47	285.82	290.62	290.32	291.14	290.19
H_2O	O	535.90	536.77	530.02	537.91	536.85	539.08	537.76
H_2O	O	537.00	538.31	533.42	539.00	537.93	540.28	539.35
MAE			1.59	3.96	1.54	1.34	3.55	2.51

Table S3: Excitation energies (in eV) for 28 K-edge transitions from Ref. 1, including some higher-lying transitions, computed at the ΔSCF level using B3LYP in two different basis sets. All theoretical calculations include relativistic corrections.

Molecule	Atom	Transition	Expt.	ΔSCF (B3LYP)		
				def2-QZVPD	double-aug.[a]	diff.[b]
NH_3	N	$1s \rightarrow 3s$	400.66	400.57	400.49	0.08
NH_3	N	$1s \rightarrow 3p(E)$	402.33	402.30	402.09	0.21
NH_3	N	$1s \rightarrow 3p(A_1)$	402.86	402.35	402.12	0.23
NH_3	N	$1s \rightarrow 4s(A_1)$	403.57	403.71	403.07	0.64
HCHO (formaldehyde)	C	$1s \rightarrow \pi^*$	285.59	285.56	285.55	0.01
HCHO (formaldehyde)	C	$1s \rightarrow 3s$	290.18	290.22	290.18	0.04
HCHO (formaldehyde)	C	$1s \rightarrow 3p(B_2)$	291.25	291.82	291.06	0.76
HCHO (formaldehyde)	C	$1s \rightarrow 3p(B_1)$	291.73	291.22	291.55	−0.33
HCHO (formaldehyde)	O	$1s \rightarrow \pi^a st$	530.82	530.73	530.73	0.00
HCHO (formaldehyde)	O	$1s \rightarrow 3s$	535.43	535.51	535.44	0.07
HCHO (formaldehyde)	O	$1s \rightarrow 3p$	536.34	536.34	536.32	0.02
CO	C	$1s \rightarrow 2p\pi^*$	287.40	286.58	286.58	0.00
CO	C	$1s \rightarrow 3s\sigma$	292.37	292.86	292.77	0.09
CO	C	$1s \rightarrow 3p\pi$	293.33	293.90	293.83	0.07
CO	C	$1s \rightarrow 3p\sigma$	293.49	294.11	293.67	0.44
CO	O	$1s \rightarrow \pi^*$	534.21	533.84	533.84	0.00
CO	O	$1s \rightarrow 3s$	538.91	538.92	538.81	0.11
CO	O	$1s \rightarrow 3p\pi$	539.91	539.98	539.86	0.12
N_2	N	$1s \rightarrow 2p\pi_g$	401.00	400.45	400.45	0.00
N_2	N	$1s \rightarrow 3s\sigma_g$	406.10	406.76	406.32	0.44
N_2	N	$1s \rightarrow 3p\pi_u$	407.00	407.72	407.31	0.41
N_2O	NC	$1s \rightarrow 3p\pi^*$	404.70	404.01	404.01	0.00
N_2O	NC	$1s \rightarrow 3p\sigma$	407.60	407.99	407.92	0.07
C_2H_4 (ethylene)	C	$1s \rightarrow \pi^*$	284.67	284.72	284.71	0.01
C_2H_4 (ethylene)	C	$1s \rightarrow 3s$	287.24	287.32	287.23	0.09
C_2H_4 (ethylene)	C	$1s \rightarrow 3p\pi$	287.88	288.09	287.95	0.14
H_2O	O	$1s \rightarrow 4a_1/3s$	534.00	533.89	533.84	0.05
H_2O	O	$1s \rightarrow 3p(b_2)$	537.00	537.14	536.92	0.22
MAE				0.31	0.25	0.17[c]

[a] def2-QZVPD with additional s and p functions on non-hydrogen atoms, whose exponents are scaled by 1/3 relative to the most diffuse s and p exponents in def2-QZVPD. [b] Difference in the excitation energies computed in the two basis sets. [c] Mean absolute difference between excitation energies in either basis set.

Table S4: Excitation energies (in eV) for 37 K-edge (1s → LUMO) transitions computed using ΔSCF, including relativistic corrections.

Molecule	Atom	Expt.	SCAN	SCAN0	B3LYP	BH&HLYP	CAM-B3LYP	LRC-ωPBE	LRC-ωPBEh	ωB97X-V
C_2H_4	C	284.7[2]	284.5	284.5	284.7	285.1	284.6	283.6	284.0	285.0
HCHO	C	285.6[3]	285.4	285.5	285.6	286.0	285.5	284.5	284.8	285.9
C_2H_2	C	285.9[2]	285.4	285.5	285.6	286.1	285.5	284.5	284.9	285.9
C_2N_2	C	286.3[4]	285.9	286.0	286.1	286.4	286.0	285.1	285.4	286.5
HCN	C	286.4[4]	286.0	286.1	286.1	286.6	286.0	285.1	285.5	286.4
acetone	C (CO)	286.4[5]	286.1	286.2	286.1	287.9	286.1	285.2	285.5	286.5
C2H6	C	286.9[2]	286.8	287.0	286.9	287.2	287.2	286.2	286.4	287.5
CO	C	287.4[6]	286.5	286.6	286.6	287.1	286.5	285.6	285.9	286.9
CH_4	C	288[7]	286.7	286.8	286.7	287.3	286.7	286.0	286.2	287.3
MeOH	C	288[5]	288.2	288.4	288.2	288.9	288.3	287.5	287.7	288.8
HCOOH	C	288.1[5]	287.6	287.7	287.7	288.2	287.6	286.6	287.0	288.0
HCOF	C	288.2[8]	287.8	287.9	287.8	288.4	287.8	286.8	287.2	288.2
CO_2	C	290.8[9]	289.8	290.0	289.9	290.6	289.9	288.8	289.2	290.2
CF_2O	C	290.9[8]	290.2	290.3	290.2	290.9	290.2	289.1	289.5	290.5
C_2N_2	N	398.9[4]	398.5	398.6	398.6	399.1	398.6	397.7	398.0	399.1
HCN	N	399.7[4]	399.3	399.4	399.4	399.8	399.3	398.4	398.7	399.8
NH_3	N	400.8[7]	400.6	400.8	400.6	401.2	400.6	399.8	400.1	401.2
N_2	N	400.9[10]	400.5	400.5	400.5	401.1	400.4	399.5	399.8	400.9
Glycine	N	401.2[11]	401.2	401.4	401.2	401.9	401.3	400.5	400.8	402.2
Pyrrole	N	402.3[12]	402.1	402.2	402.1	403.0	402.4	401.6	401.9	402.9
Imidazole	NH	402.3[13]	402.2	402.3	402.1	403.3	402.7	401.9	402.2	403.2
N_2O	N (center)	404.6[9]	404.2	404.2	404.0	404.5	404.0	403.1	403.5	404.5
HCHO	O	530.8[3]	530.8	530.7	530.7	531.0	530.7	529.8	530.0	531.1
acetone	O	531.4[5]	531.1	531.0	531.0	531.4	531.0	530.1	530.4	531.4
HCOF	O	532.1[8]	531.9	531.8	531.8	532.1	531.8	530.8	531.1	532.2
CF_2O	O	532.7[8]	532.9	532.8	532.7	533.1	532.7	531.8	532.1	533.2
H_2O	O	534[7]	534.1	534.1	533.9	534.5	534.0	533.1	533.4	534.5
MeOH	O	534.1[5]	534.2	534.3	534.0	534.7	534.2	533.2	533.5	534.6
CO	O	534.2[6]	534.0	533.9	533.8	534.2	533.9	533.0	533.2	534.3
N_2O	O	534.6[9]	535.0	534.7	534.6	534.8	534.5	533.7	534.0	535.0
Furan	O	535.2[14]	535.1	535.1	534.9	535.4	535.0	536.4	536.6	535.5
HCOOH	OH	535.4[5]	535.4	535.4	535.2	536.4	535.8	534.8	535.2	536.2
CO_2	O	535.4[9]	535.4	535.3	535.7	536.0	535.8	534.8	535.2	536.2
F_2	F	682.2[15]	682.5	682.1	682.2	682.9	682.3	681.4	681.5	682.7
HF	F	687.4[15]	687.8	687.8	687.5	688.1	687.7	686.6	686.8	688.0
HCOF	F	687.7[8]	688.0	687.9	687.7	688.2	687.9	686.8	687.1	688.2
CF_2O	F	689.2[8]	689.7	689.5	689.3	690.5	690.2	689.1	689.5	690.6

Table S5: Excitation energies (in eV) for 37 K-edge (1s → LUMO) transitions computed using STM, including relativistic corrections.

Molecule	Atom	Expt.	SCAN	SCAN0	B3LYP	BH&HLYP	CAM-B3LYP	LRC-ωPBE	LRC-ωPBEh	ωB97X-V
C_2H_4	C	284.7	286.7	286.3	285.8	285.3	285.7	285.3	285.4	286.3
HCHO	C	285.6	287.7	287.3	286.7	286.9	286.7	286.2	286.3	287.2
C_2H_2	C	285.9	287.7	287.3	286.7	286.4	286.7	286.2	286.3	287.3
C_2N_2	C	286.3	288.4	288.0	287.3	287.4	287.3	286.9	284.7	287.9
HCN	C	286.4	288.4	288.0	287.3	287.5	287.3	286.8	286.9	287.9
acetone	C (CO)	286.4	288.4	288.0	287.3	287.4	287.3	286.9	286.9	287.8
C_2H_6	C	286.9	289.1	285.2	288.0	287.7	288.1	288.1	287.9	287.9
CO	C	287.4	288.8	288.5	287.8	288.0	287.8	287.2	287.3	288.3
CH_4	C	288.0	288.9	288.6	287.8	288.0	287.9	287.7	287.6	288.6
MeOH	C	288.0	290.6	290.3	289.4	289.7	289.5	289.3	289.3	290.3
HCOOH	C	288.1	289.9	289.5	288.8	289.0	288.8	288.3	288.4	289.3
HCOF	C	288.2	290.1	289.7	289.0	289.2	289.0	288.5	288.6	289.5
CO_2	C	290.8	292.1	291.8	291.0	291.3	291.0	290.4	290.5	294.8
CF_2O	C	290.9	292.5	292.1	291.3	291.6	291.3	290.7	290.9	291.8
C_2N_2	N	398.9	401.2	400.7	399.9	401.2	400.0	399.5	399.6	400.5
HCN	N	399.7	401.9	401.4	400.7	400.7	400.7	400.3	400.3	401.3
NH_3	N	400.8	403.1	402.7	401.8	402.0	402.0	401.7	401.7	402.7
N_2	N	400.9	403.2	402.6	401.7	401.4	401.8	401.3	401.4	402.3
Glycine	N	401.2	404.9	403.5	402.5	402.8	402.8	402.7	402.6	403.6
Pyrrole	N	402.3	404.7	404.5	403.6	403.8	403.8	403.6	403.5	404.6
Imidazole	NH	402.3	404.7	404.8	403.3	404.1	404.1	403.8	403.8	404.8
N_2O	N (center)	404.6	406.8	406.3	405.3	405.3	405.3	404.9	405.0	405.9
HCHO	O	530.8	533.6	532.8	532.0	531.8	532.1	531.7	531.6	532.6
acetone	O	531.4	533.9	533.1	532.3	532.1	532.4	531.9	531.9	532.9
HCOF	O	532.1	534.7	533.9	533.0	532.8	533.1	532.7	532.6	533.6
CF_2O	O	532.7	535.7	534.8	533.9	533.7	534.0	533.6	533.5	534.6
H_2O	O	534.0	536.9	536.4	535.3	535.4	535.5	535.2	535.1	536.2
MeOH	O	534.1	537.1	536.6	535.5	535.6	535.7	535.4	535.3	536.4
CO	O	534.2	536.8	536.0	535.1	535.0	535.2	534.9	534.8	535.8
N_2O	O	534.6	537.8	536.8	535.9	535.5	535.8	535.5	535.5	538.7
Furan	O	535.2	538.0	537.2	536.2	536.1	536.3	536.0	535.9	536.9
HCOOH	OH	535.4	538.2	537.5	536.5	537.3	537.4	537.0	536.9	538.1
CO_2	O	535.4	538.2	537.4	537.2	538.5	537.4	537.1	531.8	533.7
F_2	F	682.2	685.6	684.4	683.6	683.1	683.7	683.4	683.2	684.2
HF	F	687.4	690.8	690.1	689.0	689.0	689.2	688.7	688.5	689.7
HCOF	F	687.7	691.1	690.2	689.1	688.9	689.2	688.7	688.6	689.7
CF_2O	F	689.2	692.7	691.8	690.6	692.1	692.1	691.7	691.5	692.7

Table S6: Excitation energies (in eV) for 37 K-edge (1s → LUMO) transitions computed using GSTM, including relativistic corrections.

Molecule	Atom	Expt.	SCAN	SCAN0	B3LYP	BH&HLYP	CAM-B3LYP	LRC-ωPBE	LRC-ωPBEh	ωB97X-V
C_2H_4	C	284.7	285.4	285.2	285.1	285.0	284.9	284.2	284.5	285.4
HCHO	C	285.6	286.4	286.1	285.9	286.1	285.8	285.1	285.3	286.3
C_2H_2	C	285.9	286.3	286.1	285.9	285.9	285.8	285.2	285.4	286.3
C_2N_2	C	286.3	286.8	286.7	286.4	287.2	286.4	285.7	285.9	286.8
HCN	C	286.4	286.9	286.7	286.5	286.5	286.3	285.5	285.8	286.6
acetone	C (CO)	286.4	287.0	286.8	286.5	286.0	286.3	285.7	285.9	286.7
C_2H_6	C	286.9	287.8	287.8	287.3	287.4	287.5	286.8	286.9	287.9
CO	C	287.4	287.3	287.2	286.9	287.2	286.9	286.1	286.4	287.3
CH_4	C	288.0	287.7	287.6	287.1	287.5	287.1	286.5	286.7	287.7
MeOH	C	288.0	289.2	289.1	288.6	289.1	288.6	288.0	288.2	289.3
HCOOH	C	288.1	288.6	288.4	288.0	288.1	287.8	287.1	287.3	288.1
HCOF	C	288.2	288.7	288.5	288.2	288.5	288.1	287.4	287.6	288.6
CO_2	C	290.8	290.6	290.4	289.9	290.2	289.7	291.9	289.2	293.4
CF_2O	C	290.9	291.1	291.0	290.6	290.9	290.5	289.7	289.9	290.8
C_2N_2	N	398.9	399.6	399.3	399.0	400.8	399.0	398.3	398.5	399.5
HCN	N	399.7	400.4	400.1	399.8	399.8	399.6	398.9	399.1	400.0
NH_3	N	400.8	401.7	401.6	401.0	401.4	401.0	400.4	400.6	401.7
N_2	N	400.9	401.5	401.2	400.9	401.1	400.8	400.2	400.3	401.3
Glycine	N	401.2	402.1	403.1	401.5	402.0	402.5	401.9	402.1	402.4
Pyrrole	N	402.3	403.2	402.9	402.3	403.2	402.9	402.2	402.4	403.4
Imidazole	NH	402.3	403.2	403.0	402.4	403.5	403.1	402.5	402.7	403.6
N_2O	N (center)	404.6	405.2	404.9	404.4	404.7	404.4	403.8	404.0	404.9
HCHO	O	530.8	531.9	531.5	531.2	531.2	531.2	530.5	530.6	531.6
acetone	O	531.4	532.3	531.8	531.5	531.4	531.4	530.7	530.9	531.8
HCOF	O	532.1	533.1	532.6	532.2	532.2	532.2	531.6	531.7	532.7
CF_2O	O	532.7	534.1	533.6	533.2	533.1	533.1	532.4	532.6	533.5
H_2O	O	534.0	535.3	535.0	534.4	534.7	534.5	533.7	533.9	535.0
MeOH	O	534.1	535.5	535.2	534.5	534.8	534.6	533.8	534.0	535.0
CO	O	534.2	535.2	534.7	534.3	534.3	534.3	533.7	533.8	534.7
N_2O	O	534.6	536.1	535.5	535.1	535.0	535.0	534.4	534.6	535.5
Furan	O	535.2	536.3	536.0	535.4	535.5	535.3	534.7	534.9	535.9
HCOOH	OH	535.4	536.6	536.2	535.7	535.8	535.7	534.9	535.1	536.0
CO_2	O	535.4	536.5	536.9	535.3	537.0	536.2	535.4	535.6	536.6
F_2	F	682.2	683.8	683.0	682.7	682.9	682.7	682.2	682.1	683.1
HF	F	687.4	689.2	688.8	688.1	688.3	688.2	687.3	687.4	688.5
HCOF	F	687.7	689.3	688.8	688.3	688.4	688.4	687.6	687.7	688.7
CF_2O	F	689.2	690.9	690.4	689.8	689.9	689.9	689.1	689.2	690.1

Table S7: Excitation energies (in eV) for 37 K-edge (1s $\rightarrow$ LUMO) transitions computed using TPM, including relativistic corrections.

Molecule	Atom	Expt.	SCAN	SCAN0	B3LYP	BH&HLYP	CAM-B3LYP	LRC-ωPBE	LRC-ωPBEh	ωB97X-V
C_2H_4	C	284.7	288.0	288.6	283.4	291.1	288.9	289.3	289.1	290.5
HCHO	C	285.6	289.3	290.2	288.9	290.7	290.5	290.8	290.6	292.1
C_2H_2	C	285.9	289.1	288.1	288.5	292.6	289.9	290.4	290.2	291.5
C_2N_2	C	286.3	289.4	287.3	283.9	291.9	290.5	290.8	290.6	292.0
HCN	C	286.4	289.8	290.7	289.4	291.1	291.0	291.3	291.1	292.6
acetone	C (CO)	286.4	290.0	290.9	289.5	291.3	291.1	291.4	291.2	292.7
C_2H_6	C	286.9	291.0	291.0	289.4	291.4	290.2	291.2	290.5	291.5
CO	C	287.4	290.8	291.8	290.5	292.5	292.2	292.4	292.2	293.8
CH_4	C	288.0	291.0	290.9	289.3	289.9	290.1	290.5	290.3	291.4
MeOH	C	288.0	292.2	292.4	290.8	291.5	291.6	292.0	291.9	293.0
HCOOH	C	288.1	291.6	292.5	291.1	293.0	292.7	293.0	292.8	294.4
HCOF	C	288.2	291.8	292.8	291.4	293.4	293.1	293.3	293.1	294.7
CO_2	C	290.8	294.0	295.2	293.6	295.8	295.3	295.4	295.3	296.9
CF_2O	C	290.9	294.5	295.6	294.0	296.2	295.7	295.8	295.7	297.3
C_2N_2	N	398.9	402.2	402.8	401.6	404.2	403.1	403.5	403.2	400.4
HCN	N	399.7	403.4	404.1	402.8	404.3	404.3	404.8	404.5	406.0
NH_3	N	400.8	405.3	405.3	403.5	404.2	404.5	405.0	404.9	406.0
N_2	N	400.9	404.7	403.8	399.7	409.2	406.0	401.1	406.1	407.7
Glycine	N	401.2	404.5	405.0	403.7	404.6	404.8	405.4	405.2	406.2
Pyrrole	N	402.3	405.4	405.8	404.6	405.5	405.8	406.3	406.2	407.2
Imidazole	NH	402.3	405.5	405.9	404.7	405.9	406.1	406.6	406.4	407.5
N_2O	N (center)	404.6	408.3	409.2	407.6	409.6	409.4	409.7	409.5	411.0
HCHO	O	530.8	535.0	535.4	534.0	535.3	535.6	536.1	535.7	537.2
acetone	O	531.4	535.2	537.1	535.7	535.4	537.3	537.7	537.3	538.8
HCOF	O	532.1	536.0	536.4	534.9	536.3	536.6	537.1	536.7	538.2
CF_2O	O	532.7	537.0	537.4	535.9	537.4	537.6	538.0	537.6	539.2
H_2O	O	534.0	539.3	539.2	537.2	537.9	538.3	538.9	538.6	539.8
MeOH	O	534.1	539.0	538.9	537.0	537.7	538.1	538.6	538.4	539.5
CO	O	534.2	538.3	538.8	537.3	538.7	539.0	539.5	539.1	540.6
N_2O	O	534.6	538.5	538.8	537.3	538.6	538.9	539.4	539.0	540.5
Furan	O	535.2	538.7	538.9	537.5	538.5	539.0	539.5	539.2	540.5
HCOOH	OH	535.4	538.7	539.1	537.5	539.0	539.2	539.6	539.3	540.8
CO_2	O	535.4	539.4	539.8	538.1	541.2	539.8	540.2	534.7	541.3
F_2	F	682.2	687.3	688.1	686.4	691.2	688.3	688.5	688.2	685.5
HF	F	687.4	693.6	693.4	691.1	691.9	692.5	693.0	692.6	693.9
HCOF	F	687.7	691.5	691.8	690.1	691.5	691.9	692.2	691.8	693.4
CF_2O	F	689.2	693.1	693.5	691.7	693.8	693.5	693.8	693.4	695.1

Table S8: Excitation energies (in eV) for 37 K-edge (1s → LUMO) transitions computed using GTPM, including relativistic corrections.

Molecule	Atom	Expt.	SCAN	SCAN0	B3LYP	BH&HLYP	CAM-B3LYP	LRC-ωPBE	LRC-ωPBEh	ωB97X-V
C_2H_4	C	284.7	286.6	286.5	286.7	290.9	288.1	288.2	288.2	289.6
HCHO	C	285.6	287.8	288.9	288.1	290.1	289.7	289.7	289.6	291.2
C_2H_2	C	285.9	282.3	288.5	287.7	292.2	288.0	289.4	288.6	290.7
C_2N_2	C	286.3	287.9	288.9	284.0	291.8	287.4	289.8	289.7	289.5
HCN	C	286.4	288.4	289.4	288.6	290.3	290.0	290.1	290.0	291.4
acetone	C (CO)	286.4	288.5	289.6	288.7	289.9	290.2	290.3	290.3	291.6
C_2H_6	C	286.9	289.5	288.1	288.6	291.3	289.6	289.6	287.7	289.1
CO	C	287.4	289.2	290.6	289.7	291.9	291.4	291.3	291.3	292.9
CH_4	C	288.0	289.6	289.8	288.6	289.4	289.3	289.5	289.5	290.6
MeOH	C	288.0	290.7	291.1	289.9	291.0	290.8	291.0	291.0	292.1
HCOOH	C	288.1	290.1	291.3	290.3	292.3	291.8	291.8	291.8	293.3
HCOF	C	288.2	290.3	291.6	290.6	292.8	292.2	292.2	292.2	293.8
CO2	C	290.8	292.5	293.7	292.5	294.8	294.1	293.9	294.0	295.5
CF_2O	C	290.9	293.0	294.4	293.2	295.5	294.8	294.7	294.8	296.3
C_2N_2	N	398.9	400.6	401.5	400.7	403.5	402.2	402.3	402.2	400.6
HCN	N	399.7	401.8	402.8	401.9	403.5	403.3	403.4	403.4	404.8
NH_3	N	400.8	403.7	404.0	403.3	403.7	403.7	404.6	403.9	405.1
N_2	N	400.9	403.1	404.4	403.4	409.1	403.3	400.9	405.1	406.7
Glycine	N	401.2	403.0	403.8	402.9	403.9	403.9	404.1	404.1	405.5
Pyrrole	N	402.3	403.8	404.5	403.6	404.8	404.8	405.0	405.0	406.2
Imidazole	NH	402.3	403.9	404.6	403.7	405.1	405.0	405.2	405.2	406.4
N_2O	N (center)	404.6	406.7	407.9	406.8	409.0	408.5	408.5	408.5	410.1
HCHO	O	530.8	533.2	534.0	533.1	534.7	534.7	534.9	534.7	536.3
acetone	O	531.4	533.4	534.1	533.2	534.7	534.8	534.9	534.7	536.2
HCOF	O	532.1	534.2	535.0	534.1	535.8	535.7	535.9	535.7	537.3
CF_2O	O	532.7	535.2	536.1	535.0	536.7	536.6	536.7	536.6	538.1
H_2O	O	534.0	537.5	537.8	536.3	537.4	537.4	537.7	537.6	538.8
MeOH	O	534.1	537.1	537.8	540.6	537.1	537.1	542.6	537.3	538.5
CO	O	534.2	536.5	537.4	536.4	538.1	538.1	538.3	538.1	539.6
N_2O	O	534.6	536.7	537.5	536.5	538.1	538.0	538.2	538.1	539.6
Furan	O	535.2	537.0	537.6	536.7	537.9	538.0	538.2	538.1	539.6
HCOOH	OH	535.4	536.9	537.8	536.7	538.4	538.2	538.3	538.2	539.7
CO_2	O	535.4	537.5	538.2	537.0	540.6	538.5	538.6	538.5	536.4
F_2	F	682.2	685.3	686.6	685.4	688.5	687.3	687.1	687.1	688.8
HF	F	687.4	691.6	691.9	690.2	691.4	691.5	691.8	691.6	692.9
HCOF	F	687.7	689.6	690.4	689.2	691.0	691.0	691.0	690.8	692.4
CF_2O	F	689.2	691.3	692.1	690.8	693.6	692.5	692.5	692.4	693.9

Table S9: Excitation energies (in eV) for 37 K-edge (1s → LUMO) transitions computed using FCHM, including relativistic corrections.

Molecule	Atom	Expt.	SCAN	SCAN0	B3LYP	BH&HLYP	CAM-B3LYP	LRC-ωPBE	LRC-ωPBEh	ωB97X-V
C_2H_4	C	284.7	285.3	281.9	288.9	286.7	288.4	289.5	286.4	289.1
HCHO	C	285.6	286.5	283.4	290.2	284.9	289.9	290.8	287.7	290.6
C_2H_2	C	285.9	286.3	292.3	290.1	288.1	289.6	290.7	283.9	290.3
C_2N_2	C	286.3	287.4	283.1	289.9	287.8	290.7	291.7	288.6	291.4
HCN	C	286.4	287.4	284.1	291.2	285.7	290.8	291.8	288.7	291.6
acetone	C (CO)	286.4	287.2	283.9	290.8	288.2	290.4	291.4	288.3	291.1
C_2H_6	C	286.9	290.2	286.4	292.7	289.2	291.6	292.8	289.8	292.2
CO	C	287.4	289.5	286.4	292.5	287.4	292.4	293.1	289.9	293.4
CH_4	C	288.0	290.5	286.6	292.9	286.6	291.8	293.0	290.0	292.4
MeOH	C	288.0	290.8	287.4	293.9	287.9	293.0	294.2	291.2	293.7
HCOOH	C	288.1	288.8	285.7	292.5	287.2	292.1	293.0	290.0	292.8
HCOF	C	288.2	289.0	286.0	292.7	287.6	292.4	293.3	290.2	293.2
CO_2	C	290.8	291.5	288.7	295.1	290.3	294.9	295.7	292.7	295.6
CF_2O	C	290.9	291.5	288.6	295.1	290.1	294.9	295.6	292.7	295.5
C_2N_2	N	398.9	398.9	395.4	403.6	403.2	403.2	405.3	401.2	404.4
HCN	N	399.7	401.0	396.6	404.8	397.5	404.4	406.7	402.4	405.6
NH_3	N	400.8	404.9	400.1	407.5	399.7	406.7	409.0	404.9	407.7
N_2	N	400.9	402.5	398.3	406.4	404.1	406.1	408.2	404.0	407.4
Glycine	N	401.2	404.5	400.0	407.6	399.9	406.8	409.1	405.1	407.7
Pyrrole	N	402.3	403.8	399.2	407.4	399.8	406.8	409.0	404.9	407.7
Imidazole	NH	402.3	403.8	399.3	407.5	400.0	406.9	409.1	405.0	407.8
N_2O	N (center)	404.6	405.7	401.8	409.5	403.0	409.3	411.4	407.3	410.3
HCHO	O	530.8	533.3	527.8	537.1	528.1	536.8	540.1	534.7	538.1
acetone	O	531.4	533.8	528.1	537.4	534.6	537.1	540.3	535.0	538.2
HCOF	O	532.1	534.5	529.0	538.2	529.3	537.9	541.2	535.9	539.2
CF_2O	O	532.7	535.7	530.2	539.2	530.4	539.0	542.2	537.0	540.3
H_2O	O	534.0	539.6	533.8	542.3	533.0	541.7	545.1	539.9	542.9
MeOH	O	534.1	538.8	533.0	541.7	532.4	541.1	544.5	539.3	542.3
CO	O	534.2	536.9	531.5	540.6	531.7	540.4	543.8	538.4	541.7
N_2O	O	534.6	537.1	531.5	540.7	531.8	540.4	543.6	538.4	541.7
Furan	O	535.2	537.9	532.2	541.5	532.2	541.0	544.3	539.1	542.1
HCOOH	OH	535.4	538.2	532.8	541.9	533.2	541.7	544.9	539.6	542.9
CO_2	O	535.4	538.0	532.5	541.5	537.9	541.2	544.5	539.2	542.5
F_2	F	682.2	685.5	679.2	689.5	685.9	689.4	693.6	687.2	690.8
HF	F	687.4	695.4	688.5	698.0	687.2	697.6	702.0	695.7	699.0
HCOF	F	687.7	692.7	686.2	696.4	686.0	696.3	700.5	694.1	697.6
CF_2O	F	689.2	694.4	687.9	698.1	691.1	698.0	702.2	695.8	699.3

Table S10: Excitation energies (in eV) for 37 K-edge (1s → LUMO) transitions computed using XCHM, including relativistic corrections.

Molecule	Atom	Expt.	SCAN	SCAN0	B3LYP	BH&HLYP	CAM-B3LYP	LRC-ωPBE	LRC-ωPBEh	ωB97X-V
C_2H_4	C	284.7	283.3	277.6	285.7	279.8	281.9	281.3	278.9	280.5
HCHO	C	285.6	283.8	277.7	285.8	276.5	281.9	281.6	279.0	280.5
C_2H_2	C	285.9	283.9	278.3	286.3	280.9	282.6	282.0	279.6	281.2
C_2N_2	C	286.3	285.1	279.3	287.3	282.2	283.7	283.3	280.7	282.2
HCN	C	286.4	284.7	278.7	286.7	277.6	282.9	282.5	280.0	281.5
acetone	C (CO)	286.4	284.3	278.4	286.3	285.7	282.5	282.3	279.7	281.1
C_2H_6	C	286.9	287.7	282.8	290.2	285.5	287.3	287.2	284.3	286.7
CO	C	287.4	285.6	279.4	286.9	277.6	283.2	282.9	280.2	281.9
CH_4	C	288.0	287.8	282.9	290.3	282.6	287.4	287.2	284.4	286.7
MeOH	C	288.0	288.7	283.9	291.2	283.8	288.3	287.7	285.1	287.4
HCOOH	C	288.1	286.0	280.0	287.8	278.7	284.0	283.7	281.1	282.6
HCOF	C	288.2	286.1	280.0	287.8	278.7	284.0	283.7	281.1	282.6
CO_2	C	290.8	288.2	282.4	289.9	281.1	286.3	285.9	283.4	284.9
CF_2O	C	290.9	288.2	282.2	289.8	280.7	286.0	285.6	283.1	284.6
C_2N_2	N	398.9	398.0	391.0	400.2	389.7	396.7	397.3	393.7	395.6
HCN	N	399.7	398.3	391.3	400.5	389.8	396.8	397.5	393.8	395.8
NH_3	N	400.8	401.9	395.7	404.4	395.0	401.5	402.1	398.3	400.9
N_2	N	400.9	399.4	392.0	401.3	394.4	397.5	398.4	394.6	396.4
Glycine	N	401.2	402.4	396.4	405.0	395.7	402.1	404.7	401.1	401.3
Pyrrole	N	402.3	402.5	396.1	405.0	396.8	403.2	403.7	400.1	402.3
Imidazole	NH	402.3	402.6	396.1	405.0	397.0	403.5	404.0	400.4	402.6
N_2O	N (center)	404.6	402.9	395.7	404.8	394.0	401.1	402.0	398.3	400.0
HCHO	O	530.8	531.2	523.0	533.5	521.1	529.9	531.5	526.8	528.9
acetone	O	531.4	531.8	523.8	534.2	521.9	530.6	532.3	527.5	529.7
HCOF	O	532.1	532.7	524.4	534.8	522.4	531.2	532.9	528.1	530.2
CF_2O	O	532.7	533.8	525.6	535.9	523.4	532.2	534.0	529.2	531.3
H_2O	O	534.0	536.2	528.8	538.7	527.4	535.7	537.2	532.4	535.0
MeOH	O	534.1	536.4	529.0	538.9	527.6	535.9	537.4	532.7	535.2
CO	O	534.2	534.6	526.3	536.7	524.1	533.0	534.8	530.0	532.0
N_2O	O	534.6	536.2	527.9	538.3	525.7	534.6	536.4	531.6	533.7
Furan	O	535.2	536.7	529.1	539.1	527.4	535.7	537.4	536.9	534.9
HCOOH	OH	535.4	537.9	530.0	540.1	529.1	537.4	538.8	534.2	536.6
CO_2	O	535.4	536.4	529.9	538.4	530.6	536.9	538.5	533.8	536.2
F_2	F	682.2	683.3	672.7	684.8	674.3	681.0	684.6	678.0	680.1
HF	F	687.4	691.8	683.0	694.3	680.9	691.0	693.5	687.7	690.1
HCOF	F	687.7	692.6	683.5	694.8	681.0	691.3	694.0	688.2	690.4
CF_2O	F	689.2	694.3	685.1	696.4	685.5	693.2	695.8	690.0	692.6

Table S11: Excitation energies (in eV) for 37 K-edge (1s → LUMO) transitions computed using IP-TPM@1/2, including relativistic corrections.

Molecule	Atom	Expt.	SCAN	SCAN0	B3LYP	BH&HLYP	CAM-B3LYP	LRC-ωPBE	LRC-ωPBEh	ωB97X-V
C_2H_4	C	284.7	285.7	285.2	286.4	288.3	287.8	287.8	287.8	289.3
HCHO	C	285.6	286.9	288.2	287.8	290.0	289.4	289.2	289.2	290.9
C_2H_2	C	285.9	286.8	286.4	287.5	289.5	288.9	288.8	288.9	290.3
C_2N_2	C	286.3	287.1	285.9	282.9	289.2	289.4	289.2	289.3	290.9
HCN	C	286.4	287.5	288.9	288.4	290.5	289.9	289.8	289.8	291.4
acetone	C (CO)	286.4	287.6	288.9	288.4	290.5	289.9	289.7	289.8	291.5
C_2H_6	C	286.9	288.7	289.2	288.3	289.0	289.1	289.6	289.2	290.3
CO	C	287.4	288.5	290.1	289.5	291.9	291.2	290.8	290.9	292.7
CH_4	C	288.0	288.8	289.2	288.3	289.4	289.0	288.9	289.1	290.2
MeOH	C	288.0	289.9	290.6	289.7	290.9	290.5	290.5	290.6	291.8
HCOOH	C	288.1	289.2	290.6	290.0	292.3	291.6	291.4	291.4	293.2
HCOF	C	288.2	289.4	290.9	290.3	292.7	291.9	291.7	291.7	293.6
CO_2	C	290.8	291.7	293.4	292.5	295.2	294.2	293.8	294.0	295.8
CF2O	C	290.9	292.1	293.7	292.9	295.5	294.6	294.2	294.3	296.2
C_2N_2	N	398.9	399.7	400.8	400.3	402.3	401.8	401.7	401.7	403.4
HCN	N	399.7	400.9	402.2	401.6	403.6	403.1	403.0	403.1	404.7
NH_3	N	400.8	402.8	403.4	402.4	403.6	403.3	403.3	403.5	404.7
N_2	N	400.9	402.2	402.0	403.0	405.8	404.8	404.5	404.6	406.4
Glycine	N	401.2	402.0	403.1	402.5	403.9	403.6	403.6	403.8	405.0
Pyrrole	N	402.3	402.8	403.9	403.4	404.9	404.6	404.6	404.7	405.9
Imidazole	NH	402.3	402.9	404.0	403.5	405.2	404.8	404.9	404.9	406.2
N_2O	N (center)	404.6	405.7	407.1	406.4	408.9	408.1	407.9	408.0	409.7
HCHO	O	530.8	532.1	533.3	532.7	534.6	534.3	534.2	534.2	535.8
acetone	O	531.4	532.3	533.3	532.8	534.7	534.4	534.2	534.2	535.9
HCOF	O	532.1	533.1	534.3	533.6	535.6	535.3	535.2	535.1	536.9
CF_2O	O	532.7	534.1	535.3	534.5	536.7	536.2	536.1	536.1	537.9
H_2O	O	534.0	536.5	537.1	535.9	537.3	537.1	537.0	537.1	538.4
MeOH	O	534.1	536.1	536.8	535.7	537.0	536.8	536.8	536.9	538.1
CO	O	534.2	535.4	536.7	536.0	538.0	537.7	537.6	537.6	539.2
N_2O	O	534.6	535.6	536.7	536.0	537.9	537.6	537.5	537.5	539.1
Furan	O	535.2	535.8	536.8	536.2	537.8	537.6	537.6	537.7	539.1
HCOOH	OH	535.4	535.8	537.0	536.3	538.4	537.9	537.7	537.8	539.5
CO_2	O	535.4	536.5	537.7	536.8	539.0	538.5	538.4	538.3	539.9
F_2	F	682.2	684.1	685.7	684.9	688.6	686.8	686.4	686.5	688.3
HF	F	687.4	690.5	691.1	689.8	691.3	691.1	691.1	691.1	692.5
HCOF	F	687.7	688.3	689.5	688.7	690.8	690.5	690.2	690.2	691.9
CF_2O	F	689.2	690.0	691.2	690.3	692.0	692.1	691.8	691.8	693.7

Table S12: Excitation energies (in eV) for 37 K-edge (1s → LUMO) transitions computed using IP-TPM@1/3, including relativistic corrections.

Molecule	Atom	Expt.	SCAN	SCAN0	B3LYP	BH&HLYP	CAM-B3LYP	LRC-ωPBE	LRC-ωPBEh	ωB97X-V
C_2H_4	C	284.7	284.2	283.6	284.9	286.8	286.3	286.3	286.3	287.8
HCHO	C	285.6	285.2	286.6	285.9	288.2	287.5	287.3	287.4	289.1
C_2H_2	C	285.9	285.1	284.9	285.9	287.9	287.2	287.2	287.2	288.8
C_2N_2	C	286.3	285.5	284.2	281.5	287.8	288.2	287.7	287.7	289.7
HCN	C	286.4	285.6	287.0	286.5	288.7	288.1	287.9	288.0	289.6
acetone	C (CO)	286.4	286.0	287.3	286.8	288.9	288.3	288.1	288.2	289.8
C2H6	C	286.9	287.7	288.4	287.4	288.1	288.2	288.1	288.4	289.5
CO	C	287.4	286.3	287.8	287.2	289.7	288.9	288.6	288.7	290.5
CH_4	C	288.0	287.7	288.2	287.2	288.4	288.0	287.9	288.1	289.3
MeOH	C	288.0	288.7	289.5	288.6	290.0	289.6	289.5	289.6	290.9
HCOOH	C	288.1	287.4	288.8	288.2	290.5	289.8	289.5	289.6	291.3
HCOF	C	288.2	287.5	289.0	288.4	290.8	290.0	289.7	289.8	291.6
CO_2	C	290.8	289.7	291.3	290.4	293.1	292.2	291.8	291.9	293.7
CF_2O	C	290.9	290.1	291.7	290.9	293.5	292.6	292.2	292.3	294.2
C_2N_2	N	398.9	398.2	399.3	398.8	400.8	400.3	400.2	400.2	401.9
HCN	N	399.7	399.0	400.3	399.7	401.8	401.3	401.2	401.3	402.9
NH_3	N	400.8	401.6	402.2	401.1	402.5	402.1	402.2	402.3	403.5
N_2	N	400.9	400.0	399.8	400.9	403.6	402.5	402.3	402.4	404.2
Glycine	N	401.2	401.1	402.2	401.6	403.0	402.6	402.7	402.8	404.1
Pyrrole	N	402.3	401.7	402.7	402.2	403.8	403.5	403.5	403.6	405.0
Imidazole	NH	402.3	401.7	402.7	402.2	402.5	403.6	403.6	403.7	405.1
N_2O	N (center)	404.6	403.7	405.1	404.5	404.5	406.2	405.9	406.1	407.8
HCHO	O	530.8	530.3	531.5	530.9	532.9	532.6	532.5	532.4	534.1
acetone	O	531.4	530.8	531.9	531.3	533.2	532.9	532.8	532.8	534.4
HCOF	O	532.1	531.4	532.5	531.9	533.9	533.6	533.4	533.4	535.2
CF_2O	O	532.7	532.4	533.5	532.8	534.9	534.5	534.4	534.4	536.2
H_2O	O	534.0	535.0	535.7	534.5	536.0	535.7	535.7	535.8	537.1
MeOH	O	534.1	534.8	535.6	534.5	535.9	535.6	535.7	535.7	537.0
CO	O	534.2	533.4	534.7	534.0	536.1	535.8	535.7	535.6	537.3
N_2O	O	534.6	533.9	535.0	534.4	536.3	535.9	535.8	535.9	537.5
Furan	O	535.2	534.6	535.6	535.0	536.6	536.4	536.4	536.4	537.9
HCOOH	OH	535.4	534.4	535.6	534.9	534.7	536.5	536.4	536.4	538.1
CO_2	O	535.4	534.7	535.9	535.1	537.8	536.7	536.6	536.6	538.2
F_2	F	682.2	681.6	683.2	682.5	686.1	684.4	683.9	684.0	685.9
HF	F	687.4	688.8	689.5	688.1	689.7	689.5	689.5	689.5	690.9
HCOF	F	687.7	686.9	688.0	687.3	689.4	689.0	688.8	688.8	690.5
CF_2O	F	689.2	688.5	689.7	688.8	690.5	690.6	690.4	690.3	692.2

Table S13: Excitation energies (in eV) for 37 K-edge (1s → LUMO) transitions computed using the empirically-shifted XTPM approach, including relativistic corrections.

Molecule	Atom	Expt.	SCAN	SCAN0	B3LYP	BH&HLYP	CAM-B3LYP	LRC-ωPBE	LRC-ωPBEh	ωB97X-V
C_2H_4	C	284.7	284.6	285.3	285.3	284.2	285.1	284.6	284.8	285.4
HCHO	C	285.6	285.7	286.4	286.2	285.7	286.1	285.5	285.7	286.4
C_2H_2	C	285.9	285.6	286.3	286.2	285.6	286.1	285.5	285.7	286.3
C_2N_2	C	286.3	286.1	286.7	286.8	286.7	286.6	286.1	286.5	286.7
HCN	C	286.4	286.3	286.9	286.8	286.6	286.6	286.1	286.2	286.7
acetone	C (CO)	286.4	286.3	287.1	286.8	287.1	286.7	286.2	286.4	286.9
C_2H_6	C	286.9	286.8	283.6	287.6	287.5	287.5	287.2	287.1	287.6
CO	C	287.4	286.7	287.5	287.3	286.8	287.2	286.6	286.8	287.4
CH_4	C	288.0	286.6	287.2	287.4	288.3	287.1	286.9	286.8	287.0
MeOH	C	288.0	288.2	288.8	288.9	289.9	288.7	288.4	288.3	288.6
HCOOH	C	288.1	287.9	288.6	288.3	287.9	288.2	287.6	287.8	288.3
HCOF	C	288.2	288.0	288.8	288.5	287.9	288.5	287.8	288.1	288.7
CO_2	C	290.8	290.0	290.7	290.5	290.6	290.3	292.7	292.9	292.8
CF_2O	C	290.9	290.5	291.3	290.9	291.6	290.8	290.1	290.4	291.0
C_2N_2	N	398.9	398.7	399.4	399.3	400.1	399.2	398.6	398.7	399.1
HCN	N	399.7	399.5	400.3	400.1	399.6	399.9	399.3	399.5	399.8
NH_3	N	400.8	400.5	401.2	401.2	401.9	401.0	400.7	400.6	400.8
N_2	N	400.9	400.7	401.5	401.2	399.8	401.1	400.5	400.6	401.2
Glycine	N	401.2	401.9	402.5	402.8	402.8	402.3	402.0	402.0	401.5
Pyrrole	N	402.3	402.1	402.5	403.0	403.7	402.8	402.4	402.4	402.4
Imidazole	NH	402.3	402.1	402.6	402.7	403.9	403.0	402.7	402.6	402.7
N2O	N (center)	404.6	404.4	405.2	404.7	403.7	404.6	404.1	404.2	404.8
HCHO	O	530.8	530.8	531.4	531.3	530.4	531.1	530.5	530.7	530.9
acetone	O	531.4	531.1	531.6	531.6	530.9	531.3	530.8	530.9	531.0
HCOF	O	532.1	531.9	532.4	532.4	532.9	532.1	531.6	531.7	531.9
CF_2O	O	532.7	532.8	533.4	533.3	532.5	533.0	532.5	532.6	532.7
H_2O	O	534.0	533.9	534.5	534.6	535.1	534.3	533.8	533.8	533.7
MeOH	O	534.1	534.0	534.6	534.7	535.4	534.4	534.0	533.9	533.8
CO	O	534.2	534.0	534.6	534.5	533.6	534.3	533.8	533.9	534.0
N_2O	O	534.6	534.8	535.2	535.2	534.3	534.8	534.4	534.5	534.0
Furan	O	535.2	534.9	535.5	535.5	535.4	535.1	534.7	534.8	534.8
HCOOH	OH	535.4	535.1	535.6	535.7	535.9	535.3	534.8	534.8	534.6
CO_2	O	535.4	535.3	536.7	535.6	538.5	536.2	535.7	536.4	536.5
F_2	F	682.2	682.5	683.2	682.9	680.9	682.7	682.2	682.5	682.4
HF	F	687.4	687.4	687.9	688.0	688.6	687.7	687.1	687.1	686.7
HCOF	F	687.7	687.5	687.9	688.2	688.3	687.8	687.2	687.2	686.9
CF_2O	F	689.2	689.1	689.5	689.7	690.0	689.1	688.6	688.6	688.0

Table S14: Excitation energies (in eV) for 20 higher-lying transitions computed using XCHM, including relativistic corrections.

Molecules	Orbitals	Transitions	Expt.	SCAN	SCAN0	B3LYP	BH&HLYP	CAM-B3LYP	LRC-ωPBE	LRC-ωPBEh	ωB97X-V
NH_3	N	$1s \rightarrow 3p(E)$	402.33[7]	403.92	398.99	407.27	399.30	406.40	408.49	404.40	407.22
NH_3	N	$1s \rightarrow 3p(A_1)$	402.86[7]	403.92	398.99	407.27	399.30	406.40	408.49	404.40	407.22
NH_3	N	$1s \rightarrow 4s(A_1)$	403.57[7]	405.67	400.42	408.70	400.47	407.59	409.63	405.59	408.29
HCHO (formaldehyde)	C	$1s \rightarrow 3s$	290.18[3]	288.67	284.58	291.28	284.59	290.01	290.97	288.04	290.25
HCHO (formaldehyde)	C	$1s \rightarrow 3p(B_2)$	291.25[3]	290.00	285.84	292.48	285.76	291.16	292.10	289.19	291.40
HCHO (formaldehyde)	C	$1s \rightarrow 3p(B_1)$	291.73[3]	290.20	285.98	292.80	285.95	291.38	292.22	289.31	291.53
HCHO (formaldehyde)	O	$1s \rightarrow 3s$	535.43[3]	536.34	529.82	538.94	528.73	537.70	540.71	535.61	538.30
HCHO (formaldehyde)	O	$1s \rightarrow 3p$	536.34[3]	537.25	530.75	539.91	529.69	538.63	541.60	536.51	539.22
CO	C	$1s \rightarrow 3s\sigma$	292.37[6]	291.56	287.15	293.37	286.58	292.02	292.70	289.78	295.19
CO	C	$1s \rightarrow 3p\pi$	293.33[6]	292.50	288.09	294.39	287.58	292.99	293.64	290.74	295.62
CO	C	$1s \rightarrow 3p\sigma$	293.49[6]	292.80	288.35	294.49	287.70	293.14	293.84	290.92	295.98
CO	O	$1s \rightarrow 3s$	538.91[16]	539.58	532.90	541.91	531.57	540.59	543.58	538.44	543.85
CO	O	$1s \rightarrow 3p\pi$	539.91[16]	540.62	533.92	542.99	532.62	541.64	544.61	539.49	545.00
N_2	N	$1s \rightarrow 3s\sigma_g$	406.1[17]	405.86	400.46	408.15	399.73	407.03	409.25	405.14	407.75
N_2	N	$1s \rightarrow 3p\pi_u$	407[17]	406.48	400.91	408.64	400.07	407.32	409.32	405.25	407.83
N_2O	NC	$1s \rightarrow 3p\sigma$	407.6[17]	407.17	402.30	410.11	402.43	409.16	411.28	407.26	412.23
C_2H_4 (ethylene)	C	$1s \rightarrow 3s$	287.24[18]	286.41	282.26	289.05	282.88	288.11	289.27	286.11	288.96
C_2H_4 (ethylene)	C	$1s \rightarrow 3p\pi$	287.88[18]	287.17	282.93	289.76	285.39	290.77	291.76	288.77	289.74
H_2O	O	$1s \rightarrow 2b_1/3p$	535.9[7]	538.09	532.06	541.49	531.78	540.65	543.71	538.57	541.45
H_2O	O	$1s \rightarrow 3p$ (B2)	537[7]	540.26	533.74	543.05	533.02	541.88	544.85	539.76	542.51

Table S15: Excitation energies (in eV) for 20 higher-lying transitions computed using XTPM, including relativistic corrections.

Molecules	Orbitals	Expt.	SCAN	SCAN0	B3LYP	BH&HLYP	CAM-B3LYP	LRC-ωPBE	LRC-ωPBEh	ωB97X-V
NH_3	N	402.33	405.23	405.30	404.19	405.01	405.28	405.64	405.49	406.66
NH_3	N	402.86	405.23	405.30	404.19	405.01	405.28	405.64	405.49	406.66
NH_3	N	403.57	406.54	406.35	405.26	405.90	406.18	406.45	406.34	407.45
HCHO (formaldehyde)	C	290.18	291.75	291.76	290.34	291.04	291.10	291.23	291.20	292.22
HCHO (formaldehyde)	C	291.25	293.15	293.07	291.57	292.24	292.28	292.37	292.37	293.38
HCHO (formaldehyde)	C	291.73	293.16	293.10	291.70	292.33	292.36	292.39	292.39	293.41
HCHO (formaldehyde)	O	535.43	537.77	537.26	535.67	535.89	536.47	536.68	536.49	532.61
HCHO (formaldehyde)	O	536.34	538.89	538.40	536.81	537.03	537.56	537.70	537.52	532.61
CO	C	292.37	293.20	293.17	291.71	292.39	292.35	292.19	292.27	293.24
CO	C	293.33	294.16	294.13	292.73	293.41	293.34	293.15	293.24	294.23
CO	C	293.49	294.40	294.31	292.81	293.50	293.45	293.33	293.40	294.38
CO	O	538.91	540.94	540.37	538.68	538.88	539.38	539.46	539.30	540.29
CO	O	539.91	541.91	541.35	539.74	539.94	540.42	540.48	540.32	541.31
N_2	N	406.10	408.27	406.13	406.34	410.03	407.26	402.33	407.46	408.51
N_2	N	407.00	408.77	406.51	406.81	410.35	407.53	402.33	407.54	408.55
N_2O	NC	407.60	409.85	410.17	408.33	409.62	409.44	409.64	409.59	410.70
C_2H_4 (ethylene)	C	287.24	289.23	287.15	287.85	290.62	288.55	288.82	288.75	289.73
C_2H_4 (ethylene)	C	287.88	289.78	287.63	288.38	291.06	289.02	289.21	289.16	290.13
H_2O	O	535.90	538.85	538.77	537.34	538.00	538.41	538.61	538.41	539.55
H_2O	O	537.00	540.42	539.96	538.47	538.90	539.30	539.42	539.26	540.32

Table S16: Excitation energies (in eV) for 20 higher-lying transitions computed using XGTPM, including relativistic corrections.

Molecules	Orbitals	Expt.	SCAN	SCAN0	B3LYP	BH&HLYP	CAM-B3LYP	LRC-ωPBE	LRC-ωPBEh	ωB97X-V
NH_3	N	402.33	403.83	404.20	403.38	404.44	404.39	404.49	404.51	405.70
NH_3	N	402.86	403.84	404.20	403.38	404.44	404.40	404.49	404.51	405.70
NH_3	N	403.57	405.13	405.26	404.46	405.34	405.31	405.35	405.40	406.52
HCHO (formaldehyde)	C	290.18	290.33	290.56	289.52	290.39	290.24	290.17	290.26	291.30
HCHO (formaldehyde)	C	291.25	291.65	291.82	290.74	291.58	291.41	291.30	291.41	292.45
HCHO (formaldehyde)	C	291.73	291.75	291.89	290.89	291.67	291.51	291.34	291.46	292.50
HCHO (formaldehyde)	O	535.43	536.06	535.94	534.82	535.35	535.56	535.51	535.51	536.54
HCHO (formaldehyde)	O	536.34	537.14	537.04	535.94	536.46	536.64	536.51	536.53	537.58
CO	C	292.37	291.80	291.98	290.89	291.74	291.48	291.13	291.32	293.07
CO	C	293.33	292.74	292.93	291.92	292.76	292.48	292.10	292.31	294.03
CO	C	293.49	293.10	293.21	291.99	292.84	292.59	292.27	292.46	294.18
CO	O	538.91	539.21	539.01	537.77	538.26	538.43	538.25	538.27	540.03
CO	O	539.91	540.18	539.98	538.84	539.32	539.47	539.27	539.30	541.02
N_2	N	406.10	406.65	405.91	407.16	409.82	404.44	402.11	405.09	406.32
N_2	N	407.00	407.20	406.30	407.98	410.14	404.71	402.14	405.17	406.36
N2O	NC	407.60	408.21	407.07	407.48	408.77	408.54	408.51	408.61	410.39
C_2H_4 (ethylene)	C	287.24	287.85	287.02	287.08	290.47	287.74	284.55	287.88	289.17
C_2H_4 (ethylene)	C	287.88	288.45	287.50	287.63	290.86	288.20	284.83	288.27	289.60
H_2O	O	535.90	537.11	537.38	536.45	537.37	537.42	537.31	537.32	538.48
H_2O	O	537.00	538.66	538.60	537.56	538.28	538.33	538.17	538.20	539.28

Table S17: Excitation energies (in eV) for 20 higher-lying transitions computed using IP-TPM@1/2, including relativistic corrections.

Molecules	Orbitals	Expt.	SCAN	SCAN0	B3LYP	BH&HLYP	CAM-B3LYP	LRC-ωPBE	LRC-ωPBEh	ωB97X-V
NH_3	N	400.66	404.98	405.55	404.42	405.66	405.35	405.28	405.45	406.66
NH_3	N	402.33	404.98	405.55	404.42	405.66	405.35	405.28	405.45	406.66
NH_3	N	402.86	406.39	406.63	405.61	406.59	406.32	406.16	406.37	407.49
HCHO (formaldehyde)	C	285.59	292.13	292.73	291.88	293.14	292.73	292.50	292.69	293.92
HCHO (formaldehyde)	C	290.18	293.65	294.15	293.17	294.42	293.99	293.73	293.95	295.17
HCHO (formaldehyde)	C	291.25	293.66	294.17	293.36	294.57	294.15	293.88	294.09	295.31
HCHO (formaldehyde)	O	530.82	537.62	537.90	536.86	537.74	537.71	537.53	537.67	538.78
HCHO (formaldehyde)	O	535.43	538.61	538.98	537.97	538.95	538.87	538.70	538.85	539.98
CO	C	287.40	295.05	295.51	294.56	295.74	295.24	294.68	295.00	296.22
CO	C	292.37	296.17	296.59	295.75	296.87	296.32	295.67	296.02	297.24
CO	C	293.33	296.76	297.08	295.86	296.98	296.47	295.86	296.19	297.41
CO	O	534.21	541.48	541.61	540.57	541.38	541.30	540.97	541.14	542.22
CO	O	538.91	542.62	542.70	541.81	542.56	542.43	541.98	542.19	543.26
N_2	N	401.00	409.38	408.04	408.49	410.09	409.36	401.60	409.39	410.56
N_2	N	406.10	410.50	409.00	409.49	410.94	410.16	402.12	409.99	411.12
N_2O	NC	404.70	409.47	410.72	409.63	411.47	410.95	410.73	410.97	412.38
C_2H_4 (ethylene)	C	284.67	289.08	287.92	288.73	289.89	289.44	289.32	289.50	290.58
C_2H_4 (ethylene)	C	287.24	289.94	288.67	289.42	290.53	290.08	289.86	290.08	291.16
H_2O	O	534.00	538.45	538.93	537.85	539.04	538.81	538.52	538.69	539.90
H_2O	O	535.90	539.84	540.00	539.16	540.00	539.80	539.37	539.58	540.72

Table S18: Excitation energies (in eV) for 20 higher-lying transitions computed using IP-TPM@1/3, including relativistic corrections.

Molecules	Orbitals	Expt.	SCAN	SCAN0	B3LYP	BH&HLYP	CAM-B3LYP	LRC-ωPBE	LRC-ωPBEh	ωB97X-V
NH_3	N	400.66	403.66	404.34	403.16	404.51	404.18	404.13	404.29	405.53
NH_3	N	402.33	403.66	404.34	403.16	404.51	404.18	404.13	404.29	405.53
NH_3	N	402.86	405.42	405.67	404.62	405.62	405.34	405.18	405.39	406.52
HCHO (formaldehyde)	C	285.59	290.99	291.73	290.76	292.13	291.71	291.52	291.70	292.96
HCHO (formaldehyde)	C	290.18	292.47	293.15	292.02	293.40	292.96	292.76	292.96	294.22
HCHO (formaldehyde)	C	291.25	292.67	293.22	292.36	293.63	293.21	293.01	293.20	294.44
HCHO (formaldehyde)	O	530.82	536.66	537.00	535.91	536.85	536.82	536.68	536.80	537.94
HCHO (formaldehyde)	O	535.43	537.52	537.96	536.92	537.97	537.89	537.80	537.91	539.08
CO	C	287.40	294.11	294.60	293.59	294.81	294.32	293.83	294.13	295.36
CO	C	292.37	295.35	295.77	294.88	296.01	295.47	294.85	295.20	296.42
CO	C	293.33	295.96	296.29	295.02	296.16	295.65	295.06	295.39	296.61
CO	O	534.21	540.54	540.71	539.63	540.48	540.41	540.12	540.28	541.37
CO	O	538.91	541.82	541.90	540.96	541.74	541.60	541.17	541.37	542.45
N_2	N	401.00	408.34	407.02	407.44	409.04	408.31	400.56	408.35	409.53
N_2	N	406.10	409.68	408.18	408.62	410.09	409.30	401.28	409.15	410.28
N_2O	NC	404.70	407.97	409.43	408.33	410.25	409.78	409.56	409.79	411.29
C_2H_4 (ethylene)	C	284.67	288.12	287.05	287.78	289.03	288.56	288.49	288.64	289.74
C_2H_4 (ethylene)	C	287.24	289.03	287.85	288.61	289.73	289.30	289.10	289.32	290.41
H_2O	O	534.00	537.05	537.69	536.48	537.84	537.60	537.40	537.53	538.81
H_2O	O	535.90	538.95	539.11	538.22	539.08	538.89	538.48	538.69	539.83

Table S19: Excitation energies (in eV) for 20 higher-lying transitions computed using the empirically-shifted XTPM approach, including relativistic corrections.

Molecules	Orbitals	Expt.	SCAN	SCAN0	B3LYP	BH&HLYP	CAM-B3LYP	LRC-ωPBE	LRC-ωPBEh	ωB97X-V
NH_3	N	402.33	402.62	403.55	403.47	405.03	404.03	404.36	404.11	404.18
NH_3	N	402.86	402.63	403.55	403.47	405.03	404.03	404.36	404.11	404.18
NH_3	N	403.57	403.87	404.54	404.53	405.97	404.91	405.17	404.95	404.95
HCHO (formaldehyde)	C	290.18	289.53	290.28	289.76	290.86	290.16	290.24	290.15	290.37
HCHO (formaldehyde)	C	291.25	290.89	291.56	290.99	292.06	291.34	291.38	291.31	291.53
HCHO (formaldehyde)	C	291.73	290.93	291.61	291.12	292.17	291.41	291.40	291.33	291.55
HCHO (formaldehyde)	O	535.43	534.76	535.33	534.90	535.51	535.12	535.25	535.01	536.10
HCHO (formaldehyde)	O	536.34	535.89	536.48	536.04	536.63	536.22	536.27	536.05	537.52
CO	C	292.37	290.90	291.58	291.11	292.37	291.35	291.18	291.16	291.96
CO	C	293.33	291.86	292.53	292.13	293.36	292.35	292.14	292.15	292.93
CO	C	293.49	292.16	292.79	292.21	293.48	292.46	292.32	292.30	293.07
CO	O	538.91	537.89	538.38	537.89	538.58	538.01	538.01	537.79	538.20
CO	O	539.91	538.86	539.35	538.96	539.62	539.05	539.03	538.81	539.20
N_2	N	406.10	405.66	404.88	405.67	410.62	406.13	401.51	406.21	406.26
N_2	N	407.00	406.17	405.26	406.14	410.95	406.39	401.52	406.28	406.30
N_2O	NC	407.60	407.23	408.47	407.66	409.33	408.31	408.43	408.33	409.02
C_2H_4 (ethylene)	C	287.24	286.99	286.11	287.27	291.03	287.62	287.86	287.72	288.17
C_2H_4 (ethylene)	C	287.88	287.55	286.60	287.80	291.53	288.07	288.22	288.10	288.57
H_2O	O	535.90	535.75	536.60	536.51	538.08	536.90	537.05	536.73	536.50
H_2O	O	537.00	537.19	537.68	537.61	539.06	537.77	537.86	537.55	537.25

Table S20: Excitation energies (in eV) for 20 higher-lying transitions computed using ΔSCF, including relativistic corrections.

Molecule	Atom	Expt.	SCAN	SCAN0	B3LYP	BH&HLYP	CAM-B3LYP	LRC-ωPBE	LRC-ωPBEh	ωB97X-V
NH_3	N	402.33	402.33	402.56	402.30	403.06	402.48	401.62	401.89	403.06
NH_3	N	402.86	402.40	402.60	402.35	403.08	402.50	401.64	401.91	403.07
NH_3	N	403.57	403.80	403.94	403.71	404.36	403.87	402.99	403.23	404.41
HCHO (formaldehyde)	C	290.18	290.07	290.31	290.22	290.97	290.30	289.35	289.65	290.78
HCHO (formaldehyde)	C	291.25	291.73	291.93	291.82	292.05	291.93	291.04	291.30	292.47
HCHO (formaldehyde)	C	291.73	291.10	291.37	291.22	292.57	291.38	290.49	290.77	291.94
HCHO (formaldehyde)	O	535.43	535.72	535.70	535.51	535.93	535.65	534.84	535.04	536.07
HCHO (formaldehyde)	O	536.34	536.58	536.63	536.34	537.13	536.54	535.74	535.94	537.03
CO	C	292.37	292.73	293.05	292.86	293.70	292.98	291.90	292.24	294.67
CO	C	293.33	293.73	294.11	293.90	295.02	294.10	292.97	293.32	296.04
CO	C	293.49	293.95	294.33	294.11	294.80	294.34	293.24	293.57	295.63
CO	O	538.91	539.17	539.17	538.92	539.39	539.09	538.21	538.41	540.65
CO	O	539.91	540.19	540.25	539.98	540.71	540.23	539.31	539.51	542.21
N_2	N	406.10	406.82	407.01	406.76	407.48	406.92	406.97	406.23	407.36
N_2	N	407.00	407.74	407.99	407.72	408.51	407.98	408.60	407.26	408.41
N_2O	NC	407.60	407.96	408.62	407.99	410.06	408.29	407.23	407.68	409.53
C_2H_4 (ethylene)	C	287.24	287.23	287.42	287.32	288.30	287.71	286.93	287.18	288.28
C_2H_4 (ethylene)	C	287.88	288.02	288.20	288.09	288.70	288.20	287.46	287.69	289.26
H_2O	O	535.90	535.66	535.82	535.49	536.24	535.75	534.81	535.05	536.24
H_2O	O	537.00	537.52	537.59	537.14	537.92	537.54	536.58	536.80	537.96

Table S21: Excitation energies (in eV) for 29 transitions from Ref. 1, comparing BSE@G_0W_0 results from that work to shifted-XTPM (B3LYP) and TDDFT + ΔSCF (B3LYP) from the present work, including relativistic corrections

Molecule	Atom	Transition	Expt.	shifted-XTPM	TDDFT +ΔSCF	BSE@G_0W_0
NH_3	N	$1s \to 3s$	400.66	401.13	400.69	400.02
NH_3	N	$1s \to 3p(E)$	402.33	403.47	402.34	401.67
NH_3	N	$1s \to 3p(A_1)$	402.86	403.47	402.34	401.67
NH_3	N	$1s \to 4s(A_1)$	403.57	404.53	405.25	402.83
HCHO (formaldehyde)	C	$1s \to \pi^*$	285.59	286.24	285.56	284.96
HCHO (formaldehyde)	C	$1s \to 3s$	290.18	289.76	289.39	289.92
HCHO (formaldehyde)	C	$1s \to 3p(B_2)$	291.25	290.99	290.60	290.79
HCHO (formaldehyde)	C	$1s \to 3p(B_1)$	291.73	291.12	290.90	291.42
HCHO (formaldehyde)	O	$1s \to \pi^*$	530.82	531.35	530.73	529.88
HCHO (formaldehyde)	O	$1s \to 3s$	535.43	534.90	534.80	534.93
HCHO (formaldehyde)	O	$1s \to 3p$	536.34	536.04	536.17	535.71
CO	C	$1s \to 2p\pi^*$	287.40	287.29	286.59	285.46
CO	C	$1s \to 3s\sigma$	292.37	291.11	291.72	292.08
CO	C	$1s \to 3p\pi$	293.33	292.13	292.62	293.29
CO	C	$1s \to 3p\sigma$	293.49	292.21	292.77	293.60
CO	O	$1s \to \pi^*$	534.21	534.48	533.84	532.77
CO	O	$1s \to 3s$	538.91	537.89	538.59	538.25
CO	O	$1s \to 3p\pi$	539.91	538.96	539.80	539.70
N_2	N	$1s \to 2p\pi_g$	401.00	401.21	400.45	399.93
N_2	N	$1s \to 3s\sigma_g$	406.10	405.67	406.83	406.05
N_2	N	$1s \to 3p\pi_u$	407.00	406.14	407.50	407.08
N_2O	NC	$1s \to 3p\pi^*$	404.70	404.72	404.02	403.91
N_2O	NC	$1s \to 3p\sigma$	407.60	407.66	407.39	406.53
C_2H_4 (ethylene)	C	$1s \to \pi^*$	284.67	285.32	284.72	284.04
C_2H_4 (ethylene)	C	$1s \to 3s$	287.24	287.27	287.08	287.05
C_2H_4 (ethylene)	C	$1s \to 3p\pi$	287.88	287.80	287.74	287.57
H_2O	O	$1s \to 4a_1/3s$	534.00	534.48	533.99	532.66
H_2O	O	$1s \to 2b_1/3p$	535.90	536.51	535.63	534.32
H_2O	O	$1s \to 3p(b2)$	537.00	537.61	540.01	536.25