

Table 8. Relativistic (ZORA) and non Relativistic BP/ALDA and LB94/ALDA Triplet Excitation Energies (eV) of $\text{Mo}(\text{CO})_6$. The One-electron Transitions Contributing to the TDDFT Solution Vectors and the Oscillator Strengths Refer to Relativistic BP/ALDA calculations.

State	Composition	transition energy (eV)			
		BP/ZORA	LB94/ZORA	BP/n.r.	LB94/n.r.
$3T_{1u}$	96%($2t_{2g} \rightarrow 9t_{1u}$)	3.48	3.26	3.49	3.26
a^3A_{2u}	99%($2t_{2g} \rightarrow 9t_{1u}$)	3.50	3.28	3.50	3.29
a^3T_{2u}	100%($2t_{2g} \rightarrow 9t_{1u}$)	3.56	3.34	3.57	3.35
a^3E_u	100%($2t_{2g} \rightarrow 9t_{1u}$)	3.60	3.38	3.60	3.38
b^3T_{1u}	96%($2t_{2g} \rightarrow 2t_{2u}$)	4.10	3.73	4.10	3.73
b^3E_u	100%($2t_{2g} \rightarrow 2t_{2u}$)	4.12	3.75	4.12	3.74
b^3T_{2u}	100%($2t_{2g} \rightarrow 2t_{2u}$)	4.13	3.77	4.13	3.76
a^3A_{1u}	99%($2t_{2g} \rightarrow 2t_{2u}$)	4.18	3.82	4.19	3.81
a^3E_g	100%($2t_{2g} \rightarrow 2t_{1g}$)	4.95	4.43	4.94	4.41
a^3T_{2g}	100%($2t_{2g} \rightarrow 2t_{1g}$)	5.08	4.57	5.07	4.54
a^3T_{1g}	100%($2t_{2g} \rightarrow 2t_{1g}$)	5.13	4.62	5.12	4.59
a^3A_{1g}	99%($2t_{2g} \rightarrow 3t_{2g}$)	5.28	4.80	5.16	4.68
b^3E_g	100%($2t_{2g} \rightarrow 3t_{2g}$)	5.65	5.18	5.53	5.07
b^3T_{2g}	100%($2t_{2g} \rightarrow 3t_{2g}$)	5.68	5.22	5.56	5.11
b^3T_{1g}	100%($2t_{2g} \rightarrow 3t_{2g}$)	5.91	5.46	5.78	5.34
c^3T_{1g}	99%($2t_{2g} \rightarrow 6e_g$)	6.33	6.09	6.14	5.90
c^3T_{2g}	95%($2t_{2g} \rightarrow 6e_g$)	6.35	6.13	6.16	5.93
d^3T_{2g}	98%($2t_{2g} \rightarrow 9a_{1g}$)	6.48	7.41	6.49	7.46

Table 9. Relativistic (ZORA) and non Relativistic BP/ALDA and LB94/ALDA Triplet Excitation Energies (eV) of $\text{W}(\text{CO})_6$. The One-electron Transitions Contributing to the TDDFT Solution Vectors and the Oscillator Strengths Refer to Relativistic BP/ALDA calculations.

State	Composition	transition energy (eV)			
		BP/ZORA	LB94/ZORA	BP/n.r.	LB94/n.r.
a^3T_{1u}	96%($2t_{2g} \rightarrow 9t_{1u}$)	3.37	3.19	3.43	3.22
a^3A_{2u}	99%($2t_{2g} \rightarrow 9t_{1u}$)	3.39	3.22	3.44	
a^3T_{2u}	100%($2t_{2g} \rightarrow 9t_{1u}$)	3.47	3.28	3.52	3.31
a^3E_u	100%($2t_{2g} \rightarrow 9t_{1u}$)	3.50	3.32	3.55	3.34
b^3T_{1u}	96%($2t_{2g} \rightarrow 2t_{2u}$)	4.03	3.69	4.06	3.70
b^3E_u	100%($2t_{2g} \rightarrow 2t_{2u}$)	4.05	3.71	4.09	3.72
b^3T_{2u}	100%($2t_{2g} \rightarrow 2t_{2u}$)	4.07	3.73	4.10	3.74
a^3A_{1u}	99%($2t_{2g} \rightarrow 2t_{2u}$)	4.13	3.79	4.15	3.79
a^3E_g	100%($2t_{2g} \rightarrow 2t_{1g}$)	4.91	4.41	4.89	4.36
a^3T_{2g}	100%($2t_{2g} \rightarrow 2t_{1g}$)	5.05	4.56	5.01	4.49
a^3T_{1g}	100%($2t_{2g} \rightarrow 2t_{1g}$)	5.11	4.61	5.06	4.55
a^3A_{1g}	99%($2t_{2g} \rightarrow 3t_{2g}$)	5.89	5.31	5.44	4.90
b^3E_g	100%($2t_{2g} \rightarrow 3t_{2g}$)	6.23	5.68	5.78	5.26
b^3T_{2g}	93%($2t_{2g} \rightarrow 3t_{2g}$)	6.26	5.72	5.81	5.30
b^3T_{1g}	100%($2t_{2g} \rightarrow 3t_{2g}$)	6.47	5.94	6.02	5.51
c^3T_{2g}	99%($2t_{2g} \rightarrow 9a_{1g}$)	6.56	7.35	6.58	7.48
c^3T_{1g}	53%($2t_{2g} \rightarrow 6e_g$), 40%($8t_{1u} \rightarrow 9t_{1u}$)	7.09	6.93 ^a	6.48	6.17 ^c
d^3T_{2g}	60%($8t_{1u} \rightarrow 9t_{1u}$), 35%($2t_{2g} \rightarrow 6e_g$)	7.11	6.55 ^b	6.98	6.41 ^d
e^3T_{2g}	65%($2t_{2g} \rightarrow 6e_g$), 34%($8t_{1u} \rightarrow 9t_{1u}$)	7.19	6.94 ^c	6.50	6.21 ^c
d^3T_{1g}	52%($8t_{1u} \rightarrow 9t_{1u}$), 45%($2t_{2g} \rightarrow 6e_g$)	7.21	7.15 ^b	7.00 ^b	6.43 ^e

^a 91%($2t_{2g} \rightarrow 6e_g$); ^b 84%($8t_{1u} \rightarrow 9t_{1u}$); ^c 86%($2t_{2g} \rightarrow 6e_g$); ^d 78%($8t_{1u} \rightarrow 9t_{1u}$); ^e 72%($8t_{1u} \rightarrow 9t_{1u}$), 12%($2t_{2g} \rightarrow 6e_g$);