			132	70	73	76	79	82	115	109	211	112	214	217	316	319	322	325	328	228	334	231	337	Notes
MOs :	occ:	E/eV	NH3, z	Os,(z2)	Os,(x2-y2)	Os,(xy)	Os,(xz)	Os,(yz)	N(CN),(z)	N(CN),(x)	C(CN),(x)	N(CN),(y)	C(CN),(y)	C(CN),(z)	Cr,(z2)	Cr,(x2-y2)	Cr,(xy)	Cr,(xz)	Cr,(yz)	C(CO),x	O(CO),x	C(CO),y	O(CO),x	
52	1	-11.33														-0.44								Cr/CO bonding
53	1	-11.19	-0.19	-0.10										-0.17	-0.45									Cr/CO bonding
54	1	-10.61	-0.11							-0.21	-0.14	-0.23	-0.15								0.15		0.13	
55	1	-10.5	**0.61**	0.22					0.30					0.20										$NH_3(\sigma)$
56	1	-10.36								-0.28	-0.18	0.29	0.18								0.12		-0.10	cis-$NH_3(\sigma)$/CN
57	1	-10.17					-0.12	-0.10		-0.29	-0.14	-0.23	-0.10								-0.11			cis-$NH_3(\sigma)$/CN
58	1	-9.968								-0.14		0.21									-0.10		0.11	
59	1	-9.601					0.14			0.42	0.25	0.19	0.12											cis-$NH_3(\sigma)$/CN(x)
60	1	-9.539	0.31						0.32					-0.45	-0.15									trans-NH_3/CN(σ)
61	1	-9.425						-0.15		0.22	0.13	-0.42	-0.25											cis-$NH_3(\sigma)$/CN(y)
62	1	-6.911					0.48	0.36			-0.20		-0.16					0.42	0.35		-0.16		-0.13	Cr/Os, xz,yz
63	1	-6.598					-0.15	0.10									**-0.68**	-0.13	0.16					Cr,xy/cis-CO(π)
64	1	-6.542					-0.30	0.35			0.13	0.12	-0.17				0.25	-0.34	0.46		0.14	0.11	-0.19	Cr/Os, xz,yz
65	1	-6.026					**0.56**	0.42		-0.23	-0.16	-0.17	-0.13					-0.41	-0.28	-0.12	0.17		0.12	Os, xz,yz
66	1	-5.859				**0.98**	0.10																	Os, xy
67	1	-5.566					0.46	**-0.65**		-0.14	-0.14	0.20	0.22					-0.25	0.34		0.11	0.12	-0.15	Os, xz,yz
68	0	-2.561																			0.11			CO*
69	0	-2.497		-0.13										-0.30										CO*
70	0	-2.197								-0.13	0.11	0.12						-0.14		0.29	-0.23	-0.21	0.17	CO*
71	0	-2.095																						
72	0	-1.896		-0.19						0.14	-0.18	0.06						0.21	0.10	-0.42	0.29	-0.22	0.15	
73	0	-1.865		0.10						0.14	-0.18	0.16	-0.18					0.33	0.18	**-0.56**	0.40	-0.47	0.33	
74	0	-1.676						-0.10			0.12	0.23	-0.27				0.11	-0.24	0.28	0.39	-0.27	**-0.78**	0.53	
75	0	-1.509															**-0.73**		0.10				0.02	Cr, xy*
76	0	-1.435		-0.10	**0.87**											-0.10								Os, x^2-y^2
77	0	-1.353			-0.10			-0.10		0.21	-0.23	0.28	-0.29			-0.18	-0.10	-0.21	**-0.52**	-0.19	0.11	-0.11		
78	0	-1.261	-0.15	**0.53**	0.16					-0.14	0.14				-0.43			0.21	-0.13	0.17	-0.10			Os, z^{2*}
79	0	-1.175	0.10	-0.37			0.10		-0.10	-0.24	0.26	0.13	-0.12		0.16	0.34		0.29	-0.27	0.26	-0.15			
80	0	-1.112			-0.11					-0.24	0.26					**-0.65**		0.29		0.13				Cr, x^2-y^{2*}
81	0	-0.886		0.10						-0.16	0.40				0.32			0.15		-0.27	0.16			
82	0	-0.819		-0.17						0.10			0.21	0.13	**-0.52**							-0.15		Cr, z^{2*}
83	0	-0.767											0.17		0.28	-0.11						-0.14		CN(y)*
84	0	-0.754													-0.11	-0.34								CN(x)*
85	0	-0.421	-0.24	0.44					0.12	-0.01					0.11									
86	0	-0.304					0.16	0.10		**-0.57**	**0.69**	-0.34	0.44		-0.14			0.10		-0.39	0.23	-0.19	0.11	
87	0	-0.169					-0.11	0.21			-0.40	**-0.64**	**0.80**		0.12				0.14	0.19	-0.12	-0.31	0.18	
88	0	0.222	-0.35	0.46					0.27															