Electronic Supplementary Information (ESI)

Infrared Photodissociation Spectroscopy of $M(N_2)_n^+$ (M = Y, La, Ce; n = 7-8) in the Gas Phase

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Table S1. B3LYP simulated C-O/N-N bond lengths (R_{C-O}/R_{N-N}, Å), fuzzy bond order of the CO/N_2 moieties (P_{C-O}/P_{N2}), and experimental C-O/N-N stretching vibrational frequencies (ν_{C-O}/ν_{N2}, cm^{-1}) of the $M(CO)_8^+$ and $M(N_2)_8^+$ (M = Y, La, Ce) cations and their shifts with respect to free CO/N_2 molecules.

	R_{C-O}/R_{N-N}	fuzzy bond order (deviation from free CO/N_2)	ν_{C-O}/ν_{N2}	$\Delta\nu_{C-O}/\Delta\nu_{N2}$
CO	1.1242	2.71	2143	
N_2	1.0912	3.12	2330	
$Y(CO)_8^+$	1.1250	2.55 (-0.16)	2087	56
$La(CO)_8^+$	1.1244	2.57 (-0.14)	2110	33
$Ce(CO)_8^+$	1.1246	2.57 (-0.14)	2108	35
$Y(N_2)_8^+$	1.0976	2.75 (-0.37)	2226	104
$La(N_2)_8^+$	1.0968	2.81 (-0.31)	2260	70
$Ce(N_2)_8^+$	1.0968	2.88 (-0.24)	2260	70

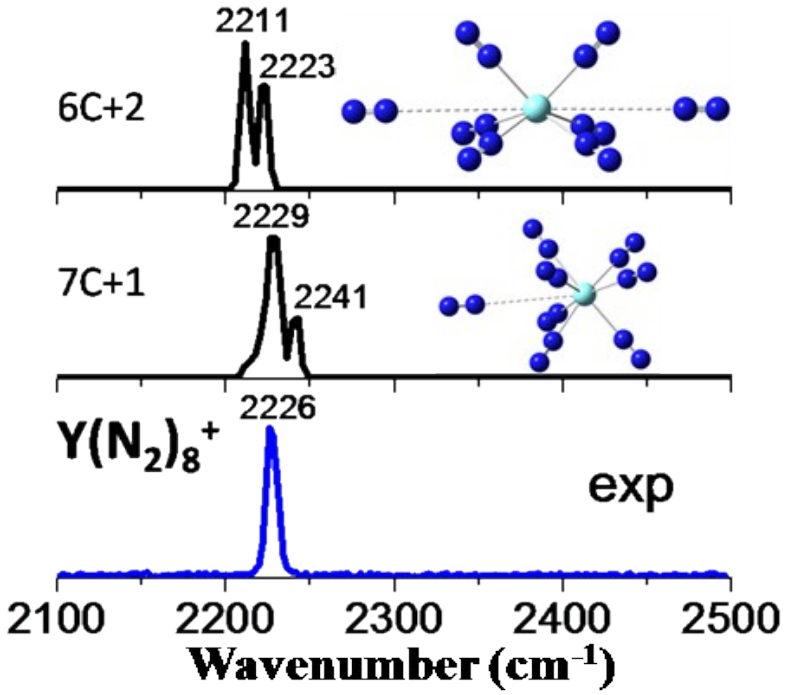

Fig. S1. Comparison of experimental IRPD spectrum with B3LYP simulated ones of (6C+2) and (7C+1) structures of $Y(N_2)_8^+$.

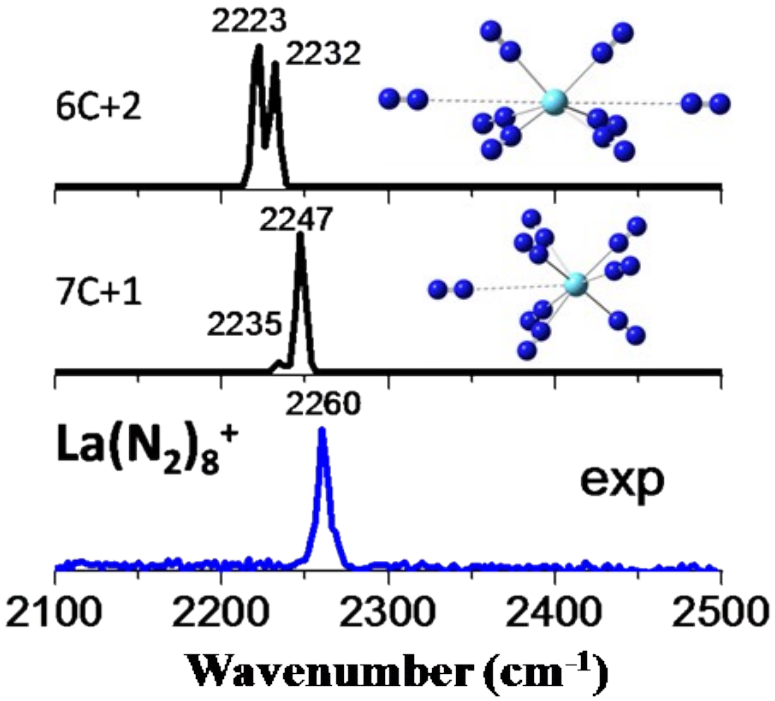

Fig. S2. Comparison of experimental IRPD spectrum with B3LYP simulated ones of (6C+2) and (7C+1) structures of $La(N_2)_8^+$.

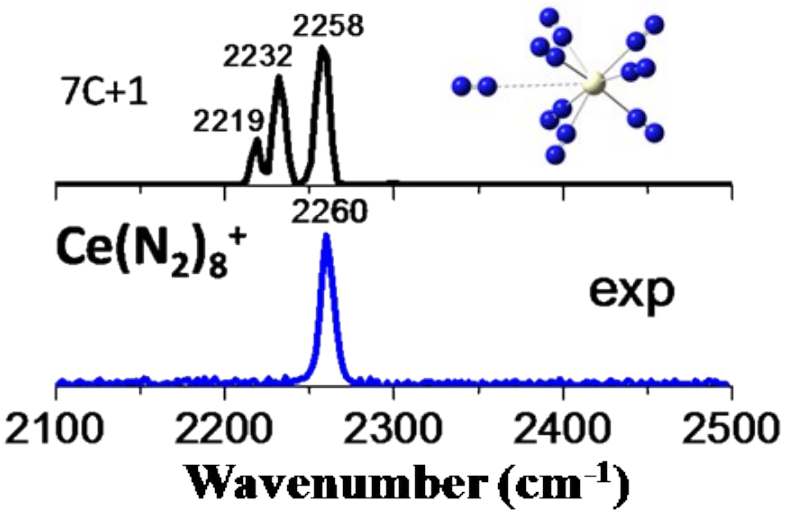

Fig. S3. Comparison of experimental IRPD spectrum with B3LYP simulated one of (7C+1) structure of $Ce(N_2)_8^+$.