Supporting Information

Infrared Photodissociation Spectroscopy of Heterodinuclear Iron-Zinc and Cobalt-Zinc Carbonyl Cation Complexes

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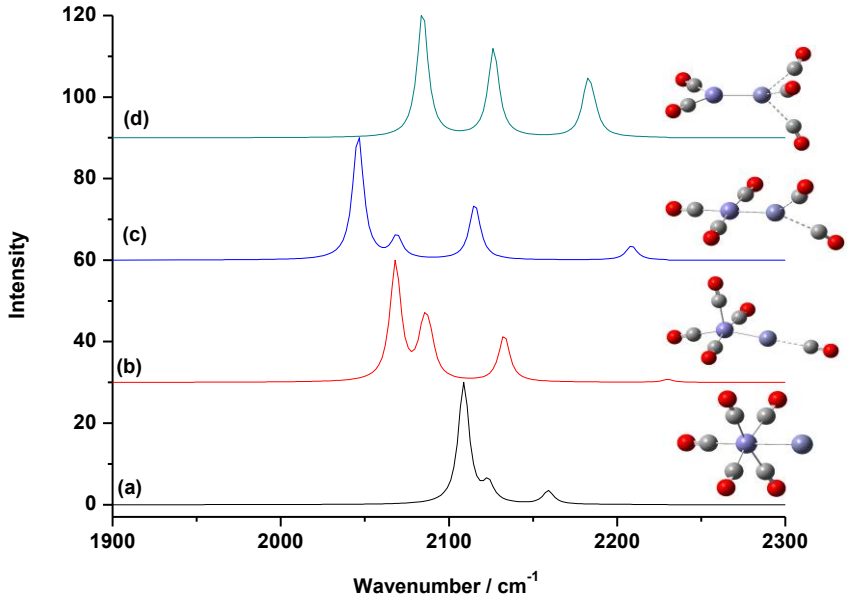

Figure S1. Simulated vibrational spectra of the $FeZn(CO)_5^+$ cation isomers (shown in Figure 3) in the carbonyl stretching frequency region.

Table S1. The Cartesian Coordinates (Å) of the Structures Optimized at the B3LYP/6-311+G(d) Level.

$FeZn(CO)_5^+$ (a)	Fe	0.000000	0.000000	-0.494533
	Zn	0.000000	0.000000	2.349633
	C	0.000000	1.871760	-0.311588
	C	-1.871760	0.000000	-0.311588
	C	0.000000	0.000000	-2.435231
	C	0.000000	-1.871760	-0.311588
	C	1.871760	0.000000	-0.311588
	O	0.000000	2.996992	-0.220065
	O	-2.996992	0.000000	-0.220065
	O	0.000000	0.000000	-3.562444
	O	0.000000	-2.996992	-0.220065
	O	2.996992	0.000000	-0.220065
$FeZn(CO)_5^+$ (b)	Fe	0.904507	-0.000015	0.138343
	C	1.305458	0.000274	-1.713575
	C	0.761170	-1.845212	0.268526
	C	2.622335	-0.000231	0.853832
	C	0.761323	1.845175	0.268906
	O	1.552562	0.000498	-2.818262
	O	0.702027	-2.975228	0.339904
	O	3.670374	-0.000400	1.278697
	O	0.702306	2.975179	0.340549
	Zn	-1.511398	-0.000007	0.127317
	C	-3.925268	0.000005	0.104291
	O	-5.042938	0.000017	0.095575
$FeZn(CO)_5^+$ (c)	Fe	-1.355890	0.001989	-0.005338
	Zn	1.081019	0.009841	-0.003692
	C	-3.202087	-0.003930	-0.006702
	C	-1.237280	1.681454	0.768309
	C	-1.225158	-1.678540	-0.771236
	C	2.864023	-1.290060	1.060659
	C	2.893696	1.273897	-1.048217
	O	-4.335375	-0.004230	-0.003778
	O	-1.184150	2.709848	1.247338
	O	-1.164758	-2.713551	-1.235613
	O	3.460651	-2.020245	1.664329
	O	3.506556	1.997694	-1.643195
$FeZn(CO)_5^+$ (d)	Zn	-0.836396	-0.000085	-0.003417
	Fe	1.683975	0.000018	-0.003111
	C	-2.410044	1.659205	-0.957812
	C	-2.407728	0.002056	1.915413
	C	-2.409804	-1.661835	-0.954367
	C	2.877299	-1.511402	0.001514
	C	2.877340	1.511404	0.000602
	O	-2.782458	2.577170	-1.484545
	O	-2.781697	0.004710	2.973213
	O	-2.782740	-2.581167	-1.478332
	O	3.557546	-2.414611	0.004995
	O	3.557620	2.414588	0.003580
$FeZn(CO)_6^+$	Fe	0.988770	-0.201474	0.000000
	Zn	-1.815955	-0.534937	0.000000
	C	0.639540	1.085392	1.320419
	C	0.639540	1.085392	-1.320419
	C	2.912959	0.033734	0.000000
	C	0.961294	-1.537308	-1.321523

	C	0.961294	-1.537308	1.321523
	O	0.445575	1.863150	2.116552
	O	0.445575	1.863150	-2.116552
	O	4.032195	0.170716	0.000000
	O	0.961294	-2.339363	-2.116657
	O	0.961294	-2.339363	2.116657
	C	-3.955545	1.966014	0.000000
	O	-4.868917	2.620578	0.000000
$CoZn(CO)_7^+$	Co	0.000000	0.000000	-1.322641
	Zn	0.000000	0.000000	1.024200
	C	0.000000	1.803176	-1.125036
	C	1.561596	-0.901588	-1.125036
	C	-1.561596	-0.901588	-1.125036
	O	0.000000	2.940496	-1.040444
	O	2.546544	-1.470248	-1.040444
	O	-2.546544	-1.470248	-1.040444
	C	0.000000	0.000000	-3.138759
	O	0.000000	0.000000	-4.270438
	C	0.000000	-1.935976	2.251643
	C	1.676604	0.967988	2.251643
	C	-1.676604	0.967988	2.251643
	O	0.000000	-2.995248	2.611378
	O	2.593961	1.497624	2.611378
	O	-2.593961	1.497624	2.611378