Electronic Supplementary Information for

Experimental and Theoretical Investigations of Infrared Multiple Photon Dissociation Spectra of Arginine Complexes with Zn^{2+} and Cd^{2+}

Aaron M. Chalifoux,[a] Georgia C. Boles,[a] Giel Berden,[b] Jos Oomens,[bc] and P. B. Armentrout[a]*

[a] Department of Chemistry, University of Utah, 315 South 1400 East, Room 2020, Salt Lake City, Utah 84112, United States

[b] Radboud University, FELIX Laboratory, Institute for Molecules and Materials, Toernooiveld 7c, NL-6525 ED Nijmegen, The Netherlands

[c] van't Hoff Institute for Molecular Sciences, University of Amsterdam, Science Park 904, NL-1098 XH Amsterdam, The Netherlands

∗Corresponding author, e-mail: armentrout@chem.utah.edu.

Table S1 provides relative single point energies of located high-energy $[Zn(Arg-H)]^+$ complexes. Tables S2 and S3 give the vibrational frequencies and IR intensities for the five lowest energy conformers of $[Zn(Arg-H)]^+$ and $CdCl^+(Arg)$ calculated at the B3LYP/6-311+G(d,p) and B3LYP/def2-TZVP levels of theory, respectively.

Figures S1 and S2 show select high energy conformers of $[Zn(Arg-H)]^+$ and $CdCl^+(Arg)$, respectively. Figures S3 and S4 show representative mass spectra for the IRMPD of $[Zn(Arg-H)]^+$ and $CdCl^+(Arg)$, respectively. Figure S5 shows the spectral comparison between the $CdCl^+(Arg)$ spectrum and composite fits of the two lowest energy conformers located.

Table S1 Relative enthalpies (0 K) and Gibbs energies (298 K) of high-energy $[Zn(Arg-H)]^+$ complexes[a]

structure	B3LYP	B3LYP-GD3BJ[b]	B3P86	MP2(full)
$[N,CO^-,N^{\delta},N^{\omega}]$-gcgctct	141.5 (141.7)	135.2 (136.4)	141.8 (142.0)	125.6 (125.8)
$[N^-,OH,N^{\omega\prime}]$-tgggtgcc	142.9 (139.8)	137.1 (133.9)	148.2 (144.1)	144.4 (141.4)
$[N^-,OH,N^{\omega\prime}]$-tggttcct	161.1 (156.9)	159.4 (155.6)	162.5 (158.3)	160.9 (156.5)
$[N,OH,N^{\delta},N^{\omega\prime-}]$-tggggtg	178.1 (175.3)	178.7 (176.7)	182.5 (179.7)	169.9 (167.1)
$[CO_2^-,N^{\delta},N^{\omega}]$-ggggtct	181.7 (180.6)	186.8 (185.7)	185.6 (184.5)	177.8 (176.7)
$[N^-,N^{\omega\prime}]$-tggttccc	214.6 (211.4)	214.5 (212.2)	216.1 (212.9)	214.2 (211.0)
$[N^{\omega-},N^{\omega\prime}]$-tggtttcc	253.4 (238.0)	282.2 (265.3)	267.0 (251.6)	275.0 (259.6)

[a] Relative single point energies at 0 K and 298 K Gibbs energies in parentheses calculated at the level of theory indicated using a 6-311+G(2d,2p) basis set and B3LYP/6-311+G(d,p) geometries and zero-point energy corrections. [b] Empirical dispersion corrected B3LYP-GD3BJ/6-311+G(2d,2p) values using B3LYP-GD3BJ/6-311+G(d,p) geometries and zero-point energy corrections.

Table S2 Vibrational frequencies (cm^{-1}) scaled by 0.975 and IR intensities (km/mol, in parentheses) for the five lowest energy conformers of $[Zn(Arg-H)]^+$ calculated at B3LYP/6-311+G(d,p) level of theory.[a]

[N,CO⁻,Nω′]-gggtgct		[N,CO⁻,Nω′]-ggggggt		[N,CO⁻,Nω′]-gcggttt		[CO₂⁻,Nω′]-gggtgct		[N⁻,CO,Nω′]-tgggtgct	
49	(9)	53	(<1)	49	(10)	49	(1)	53	(1)
74	(3)	77	(7)	68	(1)	75	(1)	79	(<1)
95	(1)	106	(1)	70	(6)	105	(1)	103	(<1)
133	(1)	123	(5)	113	(8)	113	(4)	128	(20)
143	(6)	145	(3)	145	(13)	138	(7)	147	(1)
162	(6)	147	(10)	149	(3)	148	(1)	167	(11)
193	(3)	190	(3)	183	(16)	165	(9)	187	(2)
231	(5)	220	(4)	218	(2)	189	(32)	205	(33)
260	(171)	246	(4)	237	(3)	226	(6)	220	(165)
271	(7)	265	(1)	270	(2)	240	(13)	256	(1)
286	(3)	303	(2)	313	(1)	274	(150)	275	(17)
312	(3)	328	(3)	324	(5)	278	(3)	297	(3)
327	(11)	370	(13)	361	(12)	292	(41)	312	(15)
344	(15)	396	(189)	399	(30)	314	(6)	338	(63)
371	(31)	422	(11)	415	(132)	351	(18)	346	(15)
381	(13)	428	(11)	446	(19)	372	(7)	365	(3)
439	(0)	453	(23)	466	(1)	416	(5)	386	(60)
451	(28)	493	(12)	509	(11)	435	(58)	436	(2)
509	(72)	528	(1)	532	(46)	446	(17)	504	(73)
550	(9)	571	(7)	548	(32)	536	(26)	529	(8)
590	(23)	**614**	**(31)**	565	(70)	554	(10)	582	(18)
617	**(86)**	**630**	**(17)**	579	(18)	583	(22)	**609**	**(52)**
630	**(27)**	**668**	**(9)**	**609**	**(105)**	**603**	**(148)**	**615**	**(104)**
666	**(20)**	**683**	**(120)**	**630**	**(37)**	**666**	**(6)**	**639**	**(27)**
679	**(5)**	**693**	**(17)**	**643**	**(72)**	**690**	**(16)**	**680**	**(11)**
714	**(13)**	**718**	**(40)**	**724**	**(11)**	**711**	**(16)**	**699**	**(67)**
727	**(16)**	**739**	**(5)**	**741**	**(17)**	**730**	**(8)**	**707**	**(38)**

[N,CO$^-$,N$^{\omega\prime}$]-gggtgct		[N,CO$^-$,N$^{\omega\prime}$]-ggggggt		[N,CO$^-$,N$^{\omega\prime}$]-gcggttt		[CO_2^-,N$^{\omega\prime}$]-gggtgct		[N$^-$,CO,N$^{\omega\prime}$]-tgggtgct	
785	**(13)**	**775**	**(2)**	**777**	**(24)**	**784**	**(22)**	**714**	**(45)**
804	**(12)**	**798**	**(26)**	**816**	**(7)**	**789**	**(148)**	**772**	**(15)**
840	**(32)**	**848**	**(26)**	**843**	**(24)**	**832**	**(12)**	**812**	**(19)**
878	**(0)**	**880**	**(3)**	**899**	**(1)**	**860**	**(47)**	**843**	**(2)**
922	**(2)**	**913**	**(9)**	**923**	**(1)**	**915**	**(3)**	**877**	**(1)**
954	**(9)**	**937**	**(<1)**	**943**	**(7)**	**944**	**(11)**	**922**	**(<1)**
1016	**(1)**	**1002**	**(8)**	**993**	**(10)**	**997**	**(4)**	**993**	**(7)**
1040	**(6)**	**1043**	**(41)**	**1045**	**(10)**	**1006**	**(2)**	**1027**	**(2)**
1050	**(5)**	**1054**	**(55)**	**1058**	**(3)**	**1051**	**(13)**	**1042**	**(3)**
1058	**(33)**	**1062**	**(16)**	**1081**	**(122)**	**1058**	**(19)**	**1059**	**(13)**
1075	**(150)**	**1063**	**(75)**	**1087**	**(33)**	**1107**	**(15)**	**1079**	**(43)**
1124	**(16)**	**1099**	**(38)**	**1106**	**(7)**	**1115**	**(20)**	**1124**	**(20)**
1145	**(33)**	**1141**	**(73)**	**1166**	**(43)**	**1162**	**(1)**	**1169**	**(245)**
1179	**(9)**	**1196**	**(12)**	**1191**	**(11)**	**1189**	**(8)**	**1182**	**(11)**
1223	**(100)**	**1220**	**(65)**	**1230**	**(187)**	**1223**	**(16)**	**1206**	**(20)**
1249	**(61)**	**1248**	**(22)**	**1232**	**(46)**	**1248**	**(19)**	**1229**	**(9)**
1266	**(99)**	**1253**	**(109)**	**1253**	**(14)**	**1266**	**(96)**	**1253**	**(23)**
1294	**(3)**	**1299**	**(2)**	**1285**	**(<1)**	**1292**	**(18)**	**1264**	**(85)**
1304	**(14)**	**1318**	**(13)**	**1300**	**(11)**	**1315**	**(4)**	**1297**	**(1)**
1330	**(3)**	**1326**	**(14)**	**1344**	**(7)**	**1332**	**(18)**	**1316**	**(11)**
1332	**(4)**	**1347**	**(7)**	**1352**	**(14)**	**1353**	**(32)**	**1325**	**(16)**
1358	**(3)**	**1367**	**(20)**	**1368**	**(1)**	**1363**	**(30)**	**1341**	**(1)**
1373	**(11)**	**1378**	**(30)**	**1373**	**(10)**	**1406**	**(25)**	**1369**	**(11)**
1419	**(74)**	**1403**	**(103)**	**1427**	**(24)**	**1417**	**(81)**	**1420**	**(96)**
1445	**(15)**	**1444**	**(32)**	**1435**	**(13)**	**1443**	**(90)**	**1423**	**(67)**
1463	**(15)**	**1449**	**(3)**	**1456**	**(40)**	**1453**	**(128)**	**1450**	**(22)**
1481	**(18)**	**1468**	**(18)**	**1477**	**(30)**	**1473**	**(61)**	**1465**	**(13)**
1568	**(300)**	**1537**	**(194)**	**1521**	**(148)**	**1486**	**(24)**	**1481**	**(28)**

[N,CO$^-$,N$^{\omega\prime}$]-gggtgct		[N,CO$^-$,N$^{\omega\prime}$]-gggggggt		[N,CO$^-$,N$^{\omega\prime}$]-gcggttt		[CO$_2^-$,N$^{\omega\prime}$]-gggtgct		[N$^-$,CO,N$^{\omega\prime}$]-tgggtgct	
1591	**(132)**	**1581**	**(158)**	**1567**	**(256)**	**1559**	**(282)**	**1571**	**(282)**
1606	**(76)**	**1603**	**(54)**	**1602**	**(66)**	**1593**	**(139)**	**1591**	**(159)**
1632	**(439)**	**1635**	**(447)**	**1637**	**(378)**	**1630**	**(397)**	**1630**	**(450)**
1754	**(430)**	**1755**	**(421)**	**1741**	**(386)**	**1633**	**(48)**	**1653**	**(303)**
2942	(12)	2946	(11)	2938	(20)	2973	(6)	2958	(3)
2959	(12)	2958	(21)	2954	(18)	2974	(<1)	2960	(8)
2992	(10)	2973	(6)	2965	(6)	2976	(20)	2967	(23)
2996	(8)	2985	(14)	2998	(9)	3009	(10)	2989	(5)
3016	(3)	3016	(3)	3006	(4)	3018	(4)	2999	(14)
3022	(2)	3023	(2)	3006	(12)	3035	(2)	3002	(15)
3031	(12)	3027	(8)	3020	(2)	3048	(9)	3039	(10)
3377	(23)	3388	(18)	3388	(19)	3434	(9)	3490	(47)
3438	(23)	3457	(24)	3447	(30)	3495	(55)	3513	(132)
3485	(52)	3481	(54)	3461	(73)	3504	(119)	3522	(21)
3508	(149)	3491	(140)	3493	(114)	3509	(16)	3529	(71)
3529	(78)	3502	(58)	3503	(78)	3512	(95)	3625	(76)
3620	(84)	3602	(80)	3606	(84)	3618	(82)	3628	(132)

[a] Bold indicates the region of the IR spectrum included in the present experimental study.

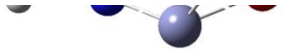
Table S3 Vibrational frequencies (cm^{-1}) scaled by 0.975 and IR intensities (km/mol, in parentheses) for the five lowest energy conformers of $CdCl^+$(Arg) calculated at B3LYP/def2-TZVP level of theory.[a]

[N,CO$^-$](N$^{\omega\prime}$H$_2^+$)-gggtgc		[N,CO,N$^{\omega\prime}$]-tgggtgct		[N,CO,N$^{\omega\prime}$]-tgtgggct		[N,CO,N$^{\omega\prime}$]-tggggggt		[N,OH,N$^{\omega\prime}$]-tgggtgct	
21	(6)	29	(2)	30	(3)	27	(5)	21	(2)
34	(<1)	38	(8)	33	(6)	31	(4)	42	(10)
50	(7)	47	(2)	50	(1)	47	(3)	49	(1)
57	(2)	62	(1)	70	(1)	60	(3)	61	(2)
74	(5)	92	(2)	88	(2)	75	(<1)	67	(4)
111	(4)	101	(5)	99	(5)	91	(7)	87	(1)
116	(10)	115	(9)	118	(4)	110	(6)	101	(4)
143	(2)	139	(5)	126	(8)	131	(1)	114	(9)
178	(19)	146	(3)	157	(2)	146	(9)	149	(<1)
189	(7)	183	(2)	196	(1)	188	(2)	185	(<1)
207	(16)	199	(6)	215	(8)	202	(2)	207	(2)
241	(37)	223	(9)	226	(<1)	208	(1)	228	(13)
249	(159)	257	(2)	233	(9)	263	(60	248	(11)
276	(8)	287	(77)	281	(66)	278	(18)	265	(81)
294	(5)	304	(5)	298	(58)	294	(5)	289	(107)
317	(21)	311	(102)	314	(90)	335	(46)	308	(23)
323	(1)	321	(74)	337	(28)	357	(180)	323	(17)
357	(34)	338	(8)	359	(2)	376	(3)	339	(16)
361	(27)	356	(10)	381	(6)	401	(24)	348	(7)
404	(3)	364	(8)	389	(43)	426	(7)	369	(6)
432	(22)	432	(17)	445	(4)	488	(17)	436	(15)
508	(31)	481	(76)	524	(12)	513	(12)	482	(76)
515	(4)	519	(15)	529	(29)	517	(9)	527	(8)
532	(103)	542	(21)	545	(21)	538	(15)	563	(41)
549	(51)	578	(10)	555	(28)	597	(2)	578	(53)

[N,CO$^-$](N$^{\omega\prime}$H$_2^+$)-gggtgc		[N,CO,N$^{\omega\prime}$]-tgggtgct		[N,CO,N$^{\omega\prime}$]-tgtgggct		[N,CO,N$^{\omega\prime}$]-tgggggggt		[N,OH,N$^{\omega\prime}$]-tgggtgct	
557	(60)	**612**	**(76)**	**623**	**(79)**	**619**	**(94)**	579	(16)
612	**(6)**	**649**	**(39)**	**642**	**(22)**	**678**	**(57)**	**646**	**(66)**
673	**(5)**	**656**	**(44)**	**659**	**(31)**	**691**	**(18)**	**649**	**(58)**
697	**(3)**	**679**	**(47)**	**668**	**(102)**	**717**	**(440**	**658**	**(3)**
724	**(17)**	**713**	**(27)**	**710**	**(21)**	**740**	**(29)**	**700**	**(28)**
749	**(6)**	**717**	**(44)**	**730**	**(46)**	**770**	**(109)**	**715**	**(15)**
820	**(28)**	**768**	**(14)**	**798**	**(10)**	**772**	**(20)**	**754**	**(9)**
835	**(46)**	**809**	**(20)**	**820**	**(6)**	**789**	**(6)**	**811**	**(9)**
888	**(6)**	**832**	**(8)**	**829**	**(13)**	**847**	**(11)**	**817**	**(2)**
906	**(5)**	**881**	**(1)**	**872**	**(6)**	**899**	**(2)**	**881**	**(5)**
944	**(3)**	**933**	**(2)**	**921**	**(1)**	**933**	**(11)**	**933**	**(2)**
997	**(79)**	**985**	**(11)**	**980**	**(19)**	**958**	**(2)**	**978**	**(11)**
1024	**(7)**	**1025**	**(124)**	**1019**	**(35)**	**1018**	**(130)**	**1036**	**(11)**
1036	**(18)**	**1036**	**(5)**	**1046**	**(33)**	**1027**	**(19)**	**1051**	**(10)**
1049	**(6)**	**1064**	**(20)**	**1061**	**(94)**	**1066**	**(3)**	**1059**	**(235)**
1053	**(55)**	**1079**	**(31)**	**1072**	**(13)**	**1067**	**(4)**	**1072**	**(15)**
1071	**(16)**	**1089**	**(7)**	**1098**	**(21)**	**1081**	**(25)**	**1080**	**(53)**
1083	**(5)**	**1145**	**(22)**	**1128**	**(8)**	**1114**	**(23)**	**1123**	**(38)**
1139	**(50)**	**1164**	**(158)**	**1154**	**(51)**	**1167**	**(211)**	**1145**	**(16)**
1164	**(14)**	**1183**	**(32)**	**1176**	**(153)**	**1183**	**(12)**	**1198**	**(13)**
1220	**(3)**	**1198**	**(7)**	**1217**	**(6)**	**1219**	**(6)**	**1202**	**(16)**
1235	**(4)**	**1248**	**(20)**	**1240**	**(21)**	**1224**	**(106)**	**1245**	**(26)**
1294	**(22)**	**1260**	**(117)**	**1253**	**(110)**	**1251**	**(8)**	**1267**	**(121)**
1319	**(13)**	**1300**	**(17)**	**1282**	**(6)**	**1298**	**(6)**	**1290**	**(2)**
1323	**(44)**	**1307**	**(6)**	**1298**	**(0)**	**1312**	**(28)**	**1307**	**(3)**
1330	**(9)**	**1320**	**(14)**	**1334**	**(18)**	**1322**	**(6)**	**1318**	**(15)**
1340	**(29)**	**1335**	**(<1)**	**1357**	**(3)**	**1350**	**(2)**	**1332**	**(5)**
1375	**(101)**	**1361**	**(2)**	**1360**	**(7)**	**1368**	**(25)**	**1361**	**(6)**

[N,CO$^-$](N$^{\omega\prime}$H$_2^+$)-gggtgc		[N,CO,N$^{\omega\prime}$]-tgggtgct		[N,CO,N$^{\omega\prime}$]-tgtgggct		[N,CO,N$^{\omega\prime}$]-tgggggggt		[N,OH,N$^{\omega\prime}$]-tgggtgct	
1380	**(66)**	**1381**	**(11)**	**1378**	**(16)**	**1382**	**(350**	**1369**	**(2)**
1416	**(29)**	**1413**	**(46)**	**1411**	**(65)**	**1392**	**(127)**	**1382**	**(16)**
1448	**(12)**	**1423**	**(95)**	**1417**	**(113)**	**1411**	**(43)**	**1424**	**(103)**
1462	**(10)**	**1451**	**(8)**	**1456**	**(14)**	**1447**	**(11)**	**1449**	**(11)**
1470	**(19)**	**1458**	**(18)**	**1461**	**(16)**	**1452**	**(9)**	**1457**	**(22)**
1575	**(61)**	**1471**	**(22)**	**1464**	**(19)**	**1465**	**(21)**	**1475**	**(13)**
1600	**(113)**	**1586**	**(322)**	**1582**	**(320)**	**1527**	**(158)**	**1586**	**(378)**
1612	**(54)**	**1591**	**(194)**	**1588**	**(174)**	**1585**	**(182)**	**1594**	**(207)**
1637	**(1088)**	**1621**	**(66)**	**1618**	**(65)**	**1610**	**(61)**	**1616**	**(62)**
1643	**(93)**	**1631**	**(343)**	**1629**	**(362)**	**1631**	**(400)**	**1634**	**(312)**
1675	**(224)**	**1709**	**(401)**	**1713**	**(404)**	**1706**	**(3950**	**1811**	**(299)**
2937	(18)	2960	(7)	2958	(4)	2968	(9)	2958	(8)
2973	(8)	2972	(7)	2970	(5)	2970	(14)	2974	(5)
2984	(10)	2980	(6)	2976	(22)	2985	(11)	2981	(3)
2987	(16)	2985	(9)	2988	(4)	2991	(4)	2992	(12)
3002	(15)	3005	(17)	2992	(12)	3012	(3)	3003	(13)
3018	(1404)	3019	(4)	3022	(7)	3024	(5)	3022	(1)
3023	(154)	3052	(13)	3063	(9)	3032	(14)	3035	(21)
3059	(4)	3372	(27)	3381	(24)	3389	(16)	3360	(25)
3385	(18)	3447	(21)	3451	(37)	3431	(30)	3426	(20)
3446	(28)	3454	(36)	3456	(24)	3457	(46)	3455	(37)
3507	(113)	3501	(115)	3499	(104)	3486	(86)	3503	(123)
3516	(83)	3525	(65)	3513	(65)	3494	(68)	3526	(73)
3551	(128)	3603	(151)	3597	(154)	3597	(63)	3602	(133)
3617	(88)	3607	(66)	3608	(64)	3600	(163)	3610	(71)

[a] Bold indicates the region of the IR spectrum included in the present experimental study.



[CO_2^-,$N^{\omega\prime}$]-gggtgcc[a]
(75.1, 83.0, 80.3, 86.2)

[CO_2^-,$N^{\omega\prime}$]-gggtgcc[a]
(83.4, 91.2, 88.1, 92.4)

[N,CO,$N^{\delta-}$,N^{ω}]-tggggtct
(111.8, 114.7, 111.1, 107.1)

[N,OH,N^{δ},$N^{\omega\prime-}$]-tggggtg
(178.1, 178.7, 182.5, 169.9)

[CO_2^-,N^{δ},N^{ω}]-ggggtct
(181.7, 186.8, 185.6, 177.8)

[N^-,$N^{\omega\prime}$]-tggttccc
(214.6, 214.5, 216.1, 214.2)

Fig. S1 Select high-energy conformers of [Zn(Arg-H)$^+$] calculated at the B3LYP/6-311G+(d,p) level of theory. Relative 0 K single point energies (in kJ/mol) at the B3LYP, B3LYP-GD3BJ, B3P86, and MP2(full)/6-311+G(2d,2p) levels of theory are given, respectively. Short dashed lines indicate hydrogen bonds. Metal-ligand interactions are shown by long dashed lines. (Red—oxygen, grey—carbon, white—hydrogen, blue—nitrogen, steel grey—zinc.) [a] These two structures are distinguished by the orientation of the NH_2 group, which hydrogen bonds to a carboxylate oxygen in the lower energy structure.

[CO,Nω′]-ctgttgcc

(49.2, 54.2, 48.6, 58.8)

[CO,Nω′]-ttgttgcc[a,b]

(63.2, 61.3, 64.4, 68.4)

[CO,Nω′]-ttgttgcc[b]

(65.6, 66.1, 68.5, 71.9)

[Nω′]-ttgttgtc

(94.4, 86.0, 100.4, 113.5)

Fig. S2 Select high-energy $CdCl^+$(Arg) conformers calculated at the B3LYP/def2-TZVP level of theory. Relative single point energies (0 K, kJ/mol) at the B3LYP, B3LYP-GD3BJ, B3P86, and MP2(full)/def2-TZVPP levels of theory are given, respectively. Short dashed lines indicate hydrogen bonds. Metal-ligand interactions are shown by long dashed lines. (Red—oxygen, grey—carbon, white—hydrogen, blue—nitrogen, yellow—cadmium, green—chlorine.) [a] This structure has a OH•Cl hydrogen bond. [b] These two structures are distinguished mainly by the orientation of the NH_2 group.

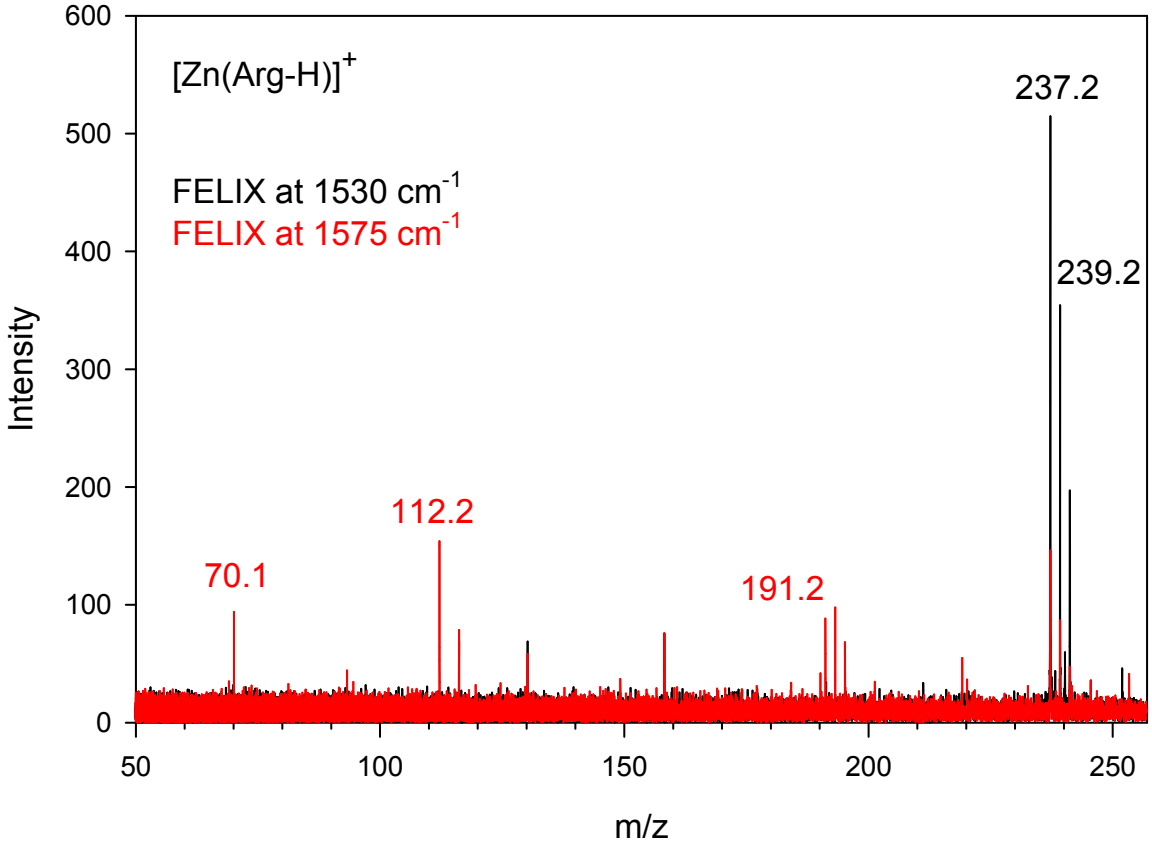


Fig. S3 Representative mass spectra for the IRMPD of $[Zn(Arg-H)]^+$. Zinc isotopes are evident in the triplet of peaks at *m/z* 239 and 191. Other unidentified peaks are noise; the result of working with low count rates in this system and a small number of averages for these spectra.

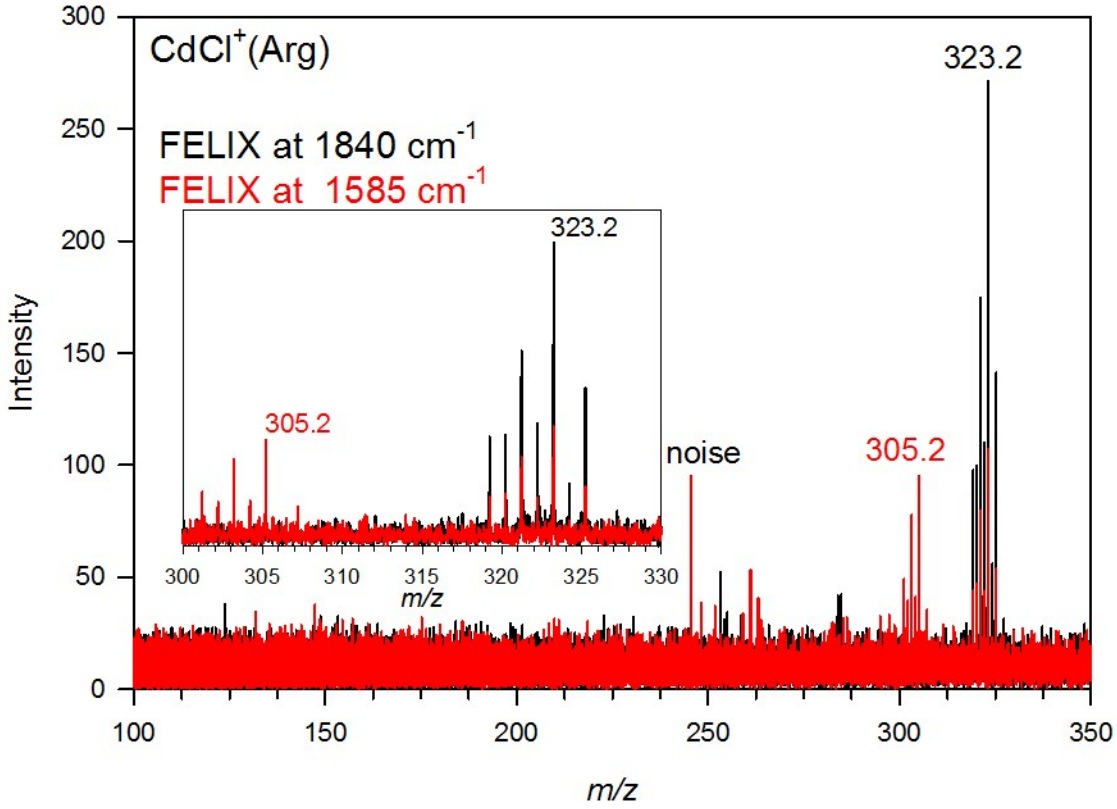


Fig. S4 Representative mass spectra for the IRMPD of $CdCl^+$(Arg). The Cd isotopes are evident in the series of peaks near *m/z* 305 and 323. Other unidentified peaks are noise; the result of working with low count rates in this system and a small number of averages for these spectra.

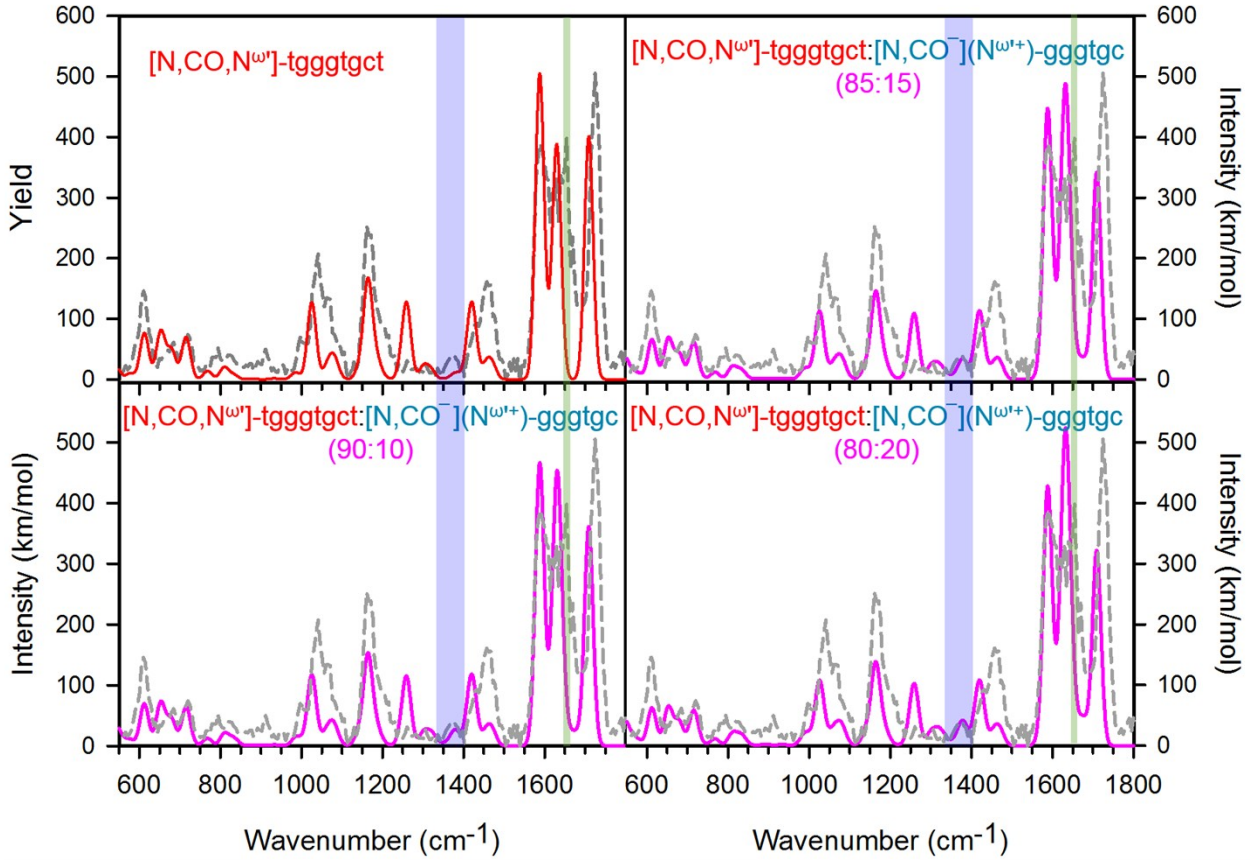


Fig. S5. Comparison of the $CdCl^+$(Arg) IRMPD spectrum (dashed grey lines) with the calculated spectrum of [N,CO,N$^{\omega}$′]-tgggtgct (red line) and composite spectra of [N,CO,N$^{\omega}$′]-tgggtgct and [N,CO$^-$](N$^{\omega'+}$)-gggtgc (pink lines) in the ratios shown. The purple and green shading highlight the peaks at 1377 and 1655 cm^{-1} that are augmented by the presence of the [N,CO$^-$](N$^{\omega'+}$)-gggtgc isomer.