Electronic Supplementary Information for

Experimental and Theoretical Investigations of the Infrared Multiple Photon Dissociation Spectroscopy of Glutamic Acid Complexes with Zn^{2+} and Cd^{2+}

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Two tables (S1 and S2) giving relative single point energies of higher energy $[Zn(Glu\text{-}H)ACN]^+$ and $CdCl^+(Glu)$ conformers calculated at the B3LYP, B3P86, and MP2(full) levels of theory from B3LYP/6-311+G(d,p) and B3LYP/def2-TZVP geometries, respectively. Two tables (S3 and S4) providing the vibrational frequencies and IR intensities for the five lowest energy conformers of $[Zn(Glu\text{-}H)ACN]^+$ and $CdCl^+(Glu)$ calculated at the B3LYP/6-311+G(d,p) and B3LYP/def2-TZVP levels of theory, respectively. Two figures S1 and S2 showing mass spectral data for the dissociation of $[Zn(Glu\text{-}H)ACN]^+$ and $CdCl^+(Glu)$, respectively. One figure S3 showing select alternate conformers of $[Zn(Glu\text{-}H)ACN]^+$. One figure S4 showing select alternate conformers of $CdCl^+(Glu)$. Two figures S5 and S6 showing a structural comparison between the observed zinc and cadmium complexes with $ZnCl^+(Glu)$ and $[Cd(Glu\text{-}H)ACN]^+$ conformers, respectively. Two figures S7 and S8 illustrating the comparison of the predicted NH and OH stretching regions of the low-energy $[Zn(Glu\text{-}H)ACN]^+$ and $CdCl^+(Glu)$ conformers likely to be formed experimentally.

Table S1. Relative Energies (0 K) and Free Energies (298 K) of Higher Energy $[Zn(Glu\text{-}H)ACN]^+$ Complexes[a]

structure	B3LYP	B3P86	MP2(full)
$[N^-,CO_s,CO]$- cggggc	84.5 (83.0)	83.2 (81.6)	85.4 (83.8)
$[N^-,C_\gamma^-,CO]$- ttgggt	86.7 (88.2)	84.5 (86.0)	91.4 (92.8)
$[C_\delta^-,CO]$- cggttt	88.3 (89.8)	86.9 (88.4)	99.4 (100.9)
$[N,CO_s,CO]$- cggggc	88.4 (89.4)	88.5 (89.5)	88.9 (89.9)
$[CO_2^-,OH_s]$- gcggt	89.5 (91.3)	94.8 (96.6)	90.3 (92.0)
$[N^-,CO]$- tgtgtt	90.9 (92.3)	95.5 (97.0)	105.2 (106.7)
$[N^-,CO_s,CO]$- cggggt	90.9 (89.9)	90.8 (89.8)	91.1 (90.0)
$[N^-,CO,OH_s]$- tggggt	93.4 (95.0)	95.1 (96.7)	86.9 (88.6)
$[N^-,CO,OH_s]$- tggggt	93.6 (95.0)	95.6 (97.0)	87.8 (89.2)
$[N^-,CO_s,OH]$- tggggt	95.8 (97.3)	99.9 (101.4)	95.2 (96.7)
$[N^-,CO_s,OH]$- tggggt	99.3 (101.5)	103.3 (105.4)	97.9 (100.0)
$[N,C_\gamma^-,CO_s]$- tgggtc	100.6 (102.2)	98.0 (99.6)	104.7 (106.3)
$[N,C_\gamma^-,CO_s]$- tgggtt	100.7 (102.4)	100.1 (101.8)	105.0 (106.7)
$[N^-,CO_s]$- ctcgtt	107.0 (105.7)	108.7 (107.3)	116.6 (115.2)
$[N^-,CO]$- cgtgtt	107.2 (108.8)	111.0 (112.6)	120.9 (122.5)
$[N^-,CO,OH_s]$- cggggt	108.2 (109.7)	109.2 (110.6)	101.4 (102.8)
$[N^-,CO_s,OH]$- tggggc	110.0 (111.7)	114.0 (115.7)	109.9 (111.6)
$[N^-,CO_s]$- cgtggt	112.6 (114.0)	115.0 (116.4)	121.8 (123.2)
$[N,C_\gamma^-,CO_s]$- cgtgtt	112.5 (114.0)	109.0 (110.4)	116.2 (117.6)
$[N^-,CO]$- tgtgtc	112.6 (115.6)	117.1 (120.1)	127.0 (130.0)
$[N,C_\gamma^-,CO_s]$- tgggtc	113.2 (114.9)	112.0 (113.7)	116.7 (118.4)
$[N,C_\gamma^-,CO_s,CO]$- cgtgtt	114.7 (116.8)	110.7 (112.8)	110.6 (112.7)
$[N^-,CO_s]$- ctcgtc	115.4 (116.5)	116.6 (117.6)	123.9 (124.9)
$[C_\gamma^-,CO,CO_s]$- cggtgc	116.9 (118.9)	112.5 (114.5)	124.6 (126.6)
$[N^-,CO_s]$- cgtggc	124.6 (125.9)	126.7 (128.0)	133.7 (135.0)
$[C_\gamma^-,CO,CO_s]$- cgggtc	125.0 (127.0)	121.0 (123.0)	128.9 (131.0)

structure	B3LYP	B3P86	MP2(full)
[N^-,CO]- cgtgtc	130.2 (132.1)	134.0 (135.9)	144.1 (146.0)
[N,C_γ^-,CO_s,CO]- cgtgtc	130.9 (133.1)	126.4 (128.6)	126.4 (128.6)
[C_β^-,CO_s,CO]- tgggtc	138.4 (141.6)	139.0 (142.1)	146.7 (149.8)
[N^-,OH,OH_s]- tggggt	141.7 (144.0)	147.2 (149.5)	131.7 (134.0)
[N^-,OH]- tttgtt	142.5 (142.3)	150.5 (150.3)	152.8 (152.6)
[N,C_γ^-,CO_s]- cgggtc	159.5 (161.9)	158.3 (160.7)	164.0 (166.4)
[N^-,OH]- tttgtc	163.3 (165.7)	171.1 (173.5)	173.5 (175.9)

[a] Relative single point energies and free energies in parentheses calculated at the level of theory indicated using a 6-311+G(2d,2p) basis set. [b] Empirical dispersion corrected B3LYP-GD3BJ values are given in bold.

Table S2. Relative Energies (0 K) and Free Energies (298 K) of Higher Energy $CdCl^+$(Glu) complexes[a]

structure	B3LYP	B3P86	MP2(full)
[N,CO,OH_s]- tgtgct	49.9 (50.0)	50.0 (50.0)	43.3 (43.3)
[CO_s,CO]- tggggt	68.4 (69.9)	74.1 (75.6)	86.8 (88.3)
[N,OH,OH_s]- tggggt	77.9 (78.4)	81.0 (81.5)	66.8 (67.3)
[N,OH_s,OH]- ttgggt	81.2 (81.5)	84.6 (85.0)	69.0 (69.3)
[N,OH_s]- tgggct	81.5 (82.3)	85.4 (86.2)	80.0 (80.8)
[N,OH,OH_s]- tgtgct	83.5 (84.0)	86.3 (86.8)	73.2 (73.7)
[N,OH]- tgtgct	86.5 (87.2)	91.3 (92.1)	88.2 (89.0)
[CO,OH_s]- tggggt	114.1 (115.7)	120.6 (122.3)	123.7 (125.3)

[a] Relative single point energies and free energies in parentheses calculated at the level of theory indicated using a def2-TZVPP basis set and SDD ECP for Cd. [b]Empirical dispersion corrected B3LYP-GD3BJ values are given in bold.

Table S3. Vibrational frequencies (cm^{-1}) scaled by 0.975 and IR intensities (km/mol, in parentheses) for the five lowest energy conformers of $[Zn(Glu\text{-}H)ACN]^+$ calculated at B3LYP/6-311+G(d,p) level of theory.[a]

$[N,CO^-,CO_s]$-gcggt		$[N,CO^-,CO_s]$-gcggc		$[N,CO^-,CO_s]$-ggggt		$[N,CO^-,CO_s]$-gtgtc		$[CO_2^-,CO_s]$-ggggt	
19	(0)	13	(0)	6	(0)	19	(0)	16	(0)
31	(3)	26	(2)	32	(2)	32	(4)	30	(3)
35	(4)	35	(7)	35	(4)	35	(7)	32	(2)
43	(5)	37	(6)	47	(8)	44	(7)	51	(1)
81	(1)	77	(1)	76	(0)	74	(1)	97	(0)
127	(1)	125	(1)	105	(2)	100	(2)	122	(2)
129	(4)	129	(4)	137	(5)	135	(4)	134	(5)
139	(1)	139	(2)	143	(11)	141	(11)	141	(14)
154	(17)	153	(30)	156	(4)	152	(4)	155	(11)
163	(19)	163	(21)	165	(15)	162	(20	179	(0)
208	(2)	209	(7)	214	(6)	213	(6)	198	(2)
223	(5)	222	(3)	229	(1)	224	(6)	213	(13)
256	(8)	256	(31)	260	(15)	266	(36)	243	(15)
293	(2)	293	(2)	298	(3)	299	(5)	257	(20)
309	(40)	309	(40)	302	(32)	303	(35)	264	(21)
355	(20)	354	(20)	348	(23)	346	(23)	315	(18)
400	(12)	400	(12)	406	(2)	406	(2)	335	(11)
407	(2)	406	(2)	408	(2)	408	(2)	361	(24)
408	(2)	408	(4)	432	(15)	434	(18)	405	(22)
440	(13)	439	(10)	447	(7)	448	(7)	408	(2)
457	(7)	463	(7)	454	(10)	458	(26)	410	(39)
542	(23)	537	(33)	554	(39)	538	(48)	443	(11)
567	(32)	553	(44)	565	(21)	564	(5)	528	(50)

[N,CO^-,CO_s]-gcggt		[N,CO^-,CO_s]-gcggc		[N,CO^-,CO_s]-ggggt		[N,CO^-,CO_s]-gtgtc		[CO_2^-,CO_s]-ggggt	
610	**(41)**	**591**	**(35)**	**603**	**(40)**	**577**	**(27)**	**586**	**(47)**
652	**(61)**	**609**	**(41)**	**623**	**(7)**	**596**	**(48)**	**651**	**(91)**
682	**(14)**	**680**	**(13)**	**653**	**(80)**	**621**	**(14)**	**673**	**(7)**
730	**(71)**	**700**	**(3)**	**742**	**(5)**	**726**	**(1)**	**753**	**(18)**
754	**(16)**	**762**	**(14)**	**752**	**(59)**	**752**	**(11)**	**768**	**(114)**
786	**(50)**	**785**	**(28)**	**788**	**(68)**	**788**	**(37)**	**773**	**(64)**
848	**(39)**	**852**	**(18)**	**846**	**(8)**	**850**	**(14)**	**820**	**(97)**
872	**(1)**	**870**	**(2)**	**866**	**(10)**	**863**	**(8)**	**859**	**(9)**
891	**(5)**	**895**	**(8)**	**908**	**(8)**	**908**	**(12)**	**910**	**(4)**
933	**(9)**	**935**	**(9)**	**934**	**(8)**	**935**	**(8)**	**937**	**(11)**
984	**(13)**	**984**	**(6)**	**961**	**(9)**	**960**	**(1)**	**965**	**(7)**
989	**(1)**	**985**	**(2)**	**1022**	**(6)**	**1023**	**(3)**	**973**	**(14)**
1024	**(7)**	**1024**	**(7)**	**1023**	**(7)**	**1023**	**(6)**	**1006**	**(30)**
1025	**(6)**	**1025**	**(6)**	**1025**	**(7)**	**1025**	**(6)**	**1023**	**(7)**
1055	**(5)**	**1055**	**(3)**	**1046**	**(20)**	**1047**	**(9)**	**1024**	**(7)**
1077	**(168)**	**1076**	**(167)**	**1080**	**(147)**	**1078**	**(138)**	**1096**	**(27)**
1155	**(32)**	**1153**	**(16)**	**1146**	**(38)**	**1143**	**(8)**	**1135**	**(40)**
1171	**(60)**	**1167**	**(8)**	**1179**	**(118)**	**1173**	**(31)**	**1190**	**(129)**
1198	**(145)**	**1189**	**(55)**	**1204**	**(75)**	**1200**	**(97)**	**1209**	**(29)**
1245	**(187)**	**1249**	**(208)**	**1225**	**(14)**	**1226**	**(103)**	**1230**	**(14)**
1264	**(24)**	**1271**	**(78)**	**1255**	**(154)**	**1258**	**(156)**	**1281**	**(10)**
1284	**(20)**	**1283**	**(140)**	**1297**	**(14)**	**1295**	**(26)**	**1298**	**(15)**
1328	**(17)**	**1316**	**(186)**	**1319**	**(11)**	**1321**	**(64)**	**1323**	**(6)**
1342	**(19)**	**1343**	**(46)**	**1338**	**(3)**	**1330**	**(141)**	**1355**	**(64)**
1352	**(27)**	**1352**	**(29)**	**1346**	**(42)**	**1342**	**(49)**	**1367**	**(9)**
1368	**(9)**	**1368**	**(9)**	**1368**	**(9)**	**1368**	**(9)**	**1385**	**(119)**
1409	**(91)**	**1387**	**(114)**	**1411**	**(94)**	**1387**	**(141)**	**1412**	**(18)**

[N,CO^-,CO_s]-gcggt		[N,CO^-,CO_s]-gcggc		[N,CO^-,CO_s]-ggggt		[N,CO^-,CO_s]-gtgtc		[CO_2^-,CO_s]-ggggt	
1414	**(18)**	**1414**	**(18)**	**1414**	**(17)**	**1414**	**(18)**	**1412**	**(18)**
1415	**(18)**	**1415**	**(18)**	**1414**	**(20)**	**1414**	**(18)**	**1424**	**(47)**
1440	**(12)**	**1439**	**(12)**	**1456**	**(14)**	**1458**	**(10)**	**1449**	**(20)**
1446	**(43)**	**1440**	**(23)**	**1465**	**(29)**	**1464**	**(16)**	**1455**	**(93)**
1605	**(65)**	**1605**	**(61)**	**1605**	**(56)**	**1606**	**(60)**	**1493**	**(193)**
1642	**(516)**	**1678**	**(355)**	**1647**	**(481)**	**1679**	**(327)**	**1624**	**(263)**
1740	**(511)**	**1738**	**(548)**	**1739**	**(538)**	**1738**	**(575)**	**1627**	**(371)**
2337	(202)	2339	(205)	2338	(207)	2339	(209)	2338	(238)
2955	(19)	2954	(20)	2969	(18)	2969	(18)	2968	(21)
2967	(4)	2961	(7)	2977	(9)	2972	(3)	2984	(4)
2969	(17)	2970	(17)	2980	(9)	2977	(11)	3003	(2)
3015	(3)	3006	(7)	3005	(3)	3003	(3)	3012	(5)
3027	(0)	3015	(3)	3031	(0)	3010	(7)	3042	(3)
3045	(7)	3028	(1)	3044	(1)	3029	(1)	3044	(8)
3045	(0)	3046	(7)	3045	(8)	3045	(8)	3045	(8)
3047	(6)	3047	(7)	3046	(7)	3047	(7)	3055	(0)
3385	(15)	3386	(16)	3389	(16)	3390	(16)	3428	(9)
3446	(26)	3448	(27)	3448	(27)	3450	(27)	3511	(15)
3624	(132)	3695	(138)	3621	(139)	3694	(140)	3630	(126)

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

Table S4. Vibrational frequencies (cm^{-1}) scaled by 0.975 and IR intensities (km/mol, in parentheses) for the five lowest energy conformers of $CdCl^+$(Glu) calculated at B3LYP/def2TZVP level of theory.[a]

[N,CO_s,CO]-tgcggt		[CO_2^-]-cgggtt		[$CO_2^-{}_s$]-ccgggt		[N,CO_s,CO]-tggggt		[N,CO]-tgtgtt	
30	(2)	21	(1)	23	(1)	33	(2)	28	(1)
41	(2)	35	(1)	39	(1)	38	(3)	35	(1)
48	(2)	46	(0)	47	(2)	46	(1)	52	(4)
67	(3)	53	(7)	59	(1)	75	(6)	60	(2)
97	(2)	61	(4)	75	(6)	82	(1)	72	(2)
110	(4)	92	(6)	90	(3)	138	(6)	96	(4)
138	(3)	102	(4)	114	(5)	143	(4)	152	(7)
153	(7)	155	(9)	166	(9)	164	(4)	167	(2)
166	(6)	206	(15)	231	(12)	187	(3)	198	(2)
215	(5)	245	(7)	261	(64)	208	(5)	221	(18)
224	(1)	273	(34	275	(0)	223	(2)	240	(0)
301	(2)	301	(60)	285	(39)	289	(1)	297	(3)
357	(38)	343	(22)	334	(87)	355	(36)	368	(36)
388	(3)	389	(21)	378	(31)	376	(14)	373	(14)
393	(15)	393	(26)	404	(3)	411	(11)	437	(7)
452	(14)	425	(7)	465	(30)	445	(11)	470	(11)
511	(22)	485	(7)	488	(39)	531	(23)	520	(37)
545	(41)	542	(34)	513	(7)	545	(19)	546	(31)
557	(16)	562	(47)	568	(25)	560	(35)	614	(85)
619	**(85)**	**600**	**(40)**	**615**	**(75)**	**597**	**(66)**	**620**	**(43)**
649	**(65)**	**631**	**(62)**	**648**	**(31)**	**651**	**(53)**	**668**	**(32)**
678	**(39)**	**689**	**(81)**	**677**	**(59)**	**669**	**(64)**	**682**	**(73)**
725	**(26)**	**763**	**(20)**	**720**	**(23)**	**721**	**(41)**	**699**	**(59)**
732	**(94)**	**793**	**(47)**	**808**	**(42)**	**746**	**(83)**	**728**	**(50)**

[N,CO_s,CO]-tgcggt		[CO_2^-]-cgggtt		[$CO_2^-{}_s$]-ccgggt		[N,CO_s,CO]-tggggt		[N,CO]-tgtgtt	
778	**(61)**	**846**	**(13)**	**838**	**(35)**	**759**	**(49)**	**795**	**(43)**
840	**(6)**	**890**	**(18)**	**897**	**(9)**	**844**	**(3)**	**843**	**(11)**
871	**(1)**	**905**	**(11)**	**916**	**(6)**	**865**	**(5)**	**892**	**(0)**
910	**(12)**	**978**	**(14)**	**986**	**(9)**	**933**	**(14)**	**918**	**(11)**
998	**(5)**	**997**	**(26)**	**1002**	**(20)**	**974**	**(4)**	**1003**	**(7)**
1011	**(20)**	**1075**	**(19)**	**1073**	**(41)**	**1030**	**(13)**	**1031**	**(11)**
1060	**(129)**	**1113**	**(14)**	**1115**	**(48)**	**1048**	**(126)**	**1059**	**(49)**
1088	**(10)**	**1147**	**(41)**	**1152**	**(176)**	**1079**	**(32)**	**1146**	**(65)**
1165	**(239)**	**1169**	**(258)**	**1161**	**(43)**	**1149**	**(88)**	**1163**	**(305)**
1169	**(87)**	**1186**	**(21)**	**1188**	**(5)**	**1172**	**(157)**	**1171**	**(159)**
1196	**(34)**	**1267**	**(31)**	**1267**	**(47)**	**1192**	**(130)**	**1202**	**(28)**
1199	**(58)**	**1285**	**(25)**	**1282**	**(27)**	**1225**	**(8)**	**1253**	**(7)**
1270	**(14)**	**1322**	**(18)**	**1322**	**(16)**	**1240**	**(3)**	**1265**	**(2)**
1292	**(10)**	**1331**	**(55)**	**1330**	**(41)**	**1306**	**(21)**	**1299**	**(60)**
1326	**(14)**	**1365**	**(41)**	**1360**	**(25)**	**1321**	**(6)**	**1333**	**(16)**
1335	**(26)**	**1403**	**(80)**	**1397**	**(21)**	**1333**	**(11)**	**1335**	**(5)**
1361	**(7)**	**1416**	**(113)**	**1415**	**(89)**	**1357**	**(19)**	**1368**	**(0)**
1410	**(18)**	**1424**	**(27)**	**1429**	**(75)**	**1405**	**(71)**	**1411**	**(19)**
1419	**(94)**	**1443**	**(35)**	**1447**	**(36)**	**1417**	**(64)**	**1414**	**(121)**
1441	**(32)**	**1489**	**(313)**	**1504**	**(484)**	**1455**	**(12)**	**1420**	**(31)**
1450	**(13)**	**1586**	**(21)**	**1531**	**(308)**	**1461**	**(19)**	**1445**	**(16)**
1617	**(74)**	**1624**	**(182)**	**1611**	**(16)**	**1617**	**(63)**	**1622**	**(101)**
1684	**(320)**	**1647**	**(30)**	**1644**	**(18)**	**1678**	**(242)**	**1696**	**(223)**
1711	**(600)**	**1694**	**(361)**	**1766**	**(246)**	**1711**	**(676)**	**1713**	**(575)**
2967	(1)	2698	(1144)	2467	(1785)	2968	(3)	2963	(1)
2979	(6)	2969	(2)	2966	(1)	2985	(3)	2972	(6)
2993	(1)	2983	(8)	2983	(7)	2994	(3)	2989	(3)

[N,CO_s,CO]-tgcggt		[CO_2^-]-cgggtt		[$CO_2^-{}_s$]-ccgggt		[N,CO_s,CO]-tggggt		[N,CO]-tgtgtt	
3027	(1)	3005	(0)	3005	(0)	3034	(1)	3020	(0)
3044	(0)	3023	(0)	3028	(1)	3047	(0)	3028	(3)
3385	(33)	3034	(1)	3031	(0)	3388	(34)	3035	(856)
3448	(35)	3229	(146)	3243	(117)	3451	(33)	3403	(48)
3590	(199)	3408	(103)	3414	(94)	3589	(129)	3591	(193)
3591	(119)	3602	(140)	3604	(165)	3596	(190)	3607	(128)

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

Figure Captions

Figure S1. Mass spectral data for the $[Zn(Glu-H)ACN]^+$ parent ion (blue) and its subsequent dissociation upon on resonance FELIX irradiation (red), with *m/z* values indicated for peaks of interest.

Figure S2. Mass spectral data for the $CdCl^+(Glu)$ parent ion (blue) and its subsequent dissociation upon on resonance FELIX irradiation (red), with *m/z* values indicated for peaks of interest.

Figure S3. Select higher energy $[Zn(Glu-H)ACN]^+$ conformers calculated at the B3LYP/6-311+G(d,p) level of theory. Relative single point enthalpies (0 K) are given at the B3LYP, B3P86, and MP2(full) levels, respectively. Short dashed lines indicate hydrogen bonds (up to 2.5 Å). Metal-ligand interactions are shown by long dashed lines.

Figure S4. Select higher energy $CdCl^+(Glu)$ conformers calculated at the B3LYP/def2-TZVP level of theory. Relative single point enthalpies (0 K) in kJ/mol are given at the B3LYP, B3P86, and MP2(full) levels, respectively. Short dashed lines indicate hydrogen bonds (up to 2.5 Å). Metal-ligand interactions are shown by long dashed lines.

Figure S5. Structural comparison between $[Zn(Glu-H)ACN]^+$ (top left), $ZnCl^+(Glu)$ (bottom left), $CdCl^+(Glu)$ (top right), and $[Cd(Glu-H)ACN]^+$ (bottom right) ground conformers. Bond lengths in Å are provided for metal-ligand bonds. Short dashed lines indicate hydrogen bonds (up to 2.5 Å). Metal-ligand interactions are shown by long dashed lines. Indicated metal-ligand interactions are given in Å.

Figure S6. Comparison of calculated spectra (B3LYP/6-311+G(d,p) level of theory) for select low-energy conformers of $[Zn(Glu-H)ACN]^+$ in the NH and OH stretching region.

Figure S7. Comparison of calculated spectra (B3LYP/def2-TZVP level of theory) for select low-energy conformers of $CdCl^+(Glu)$ in the NH and OH stretching region.

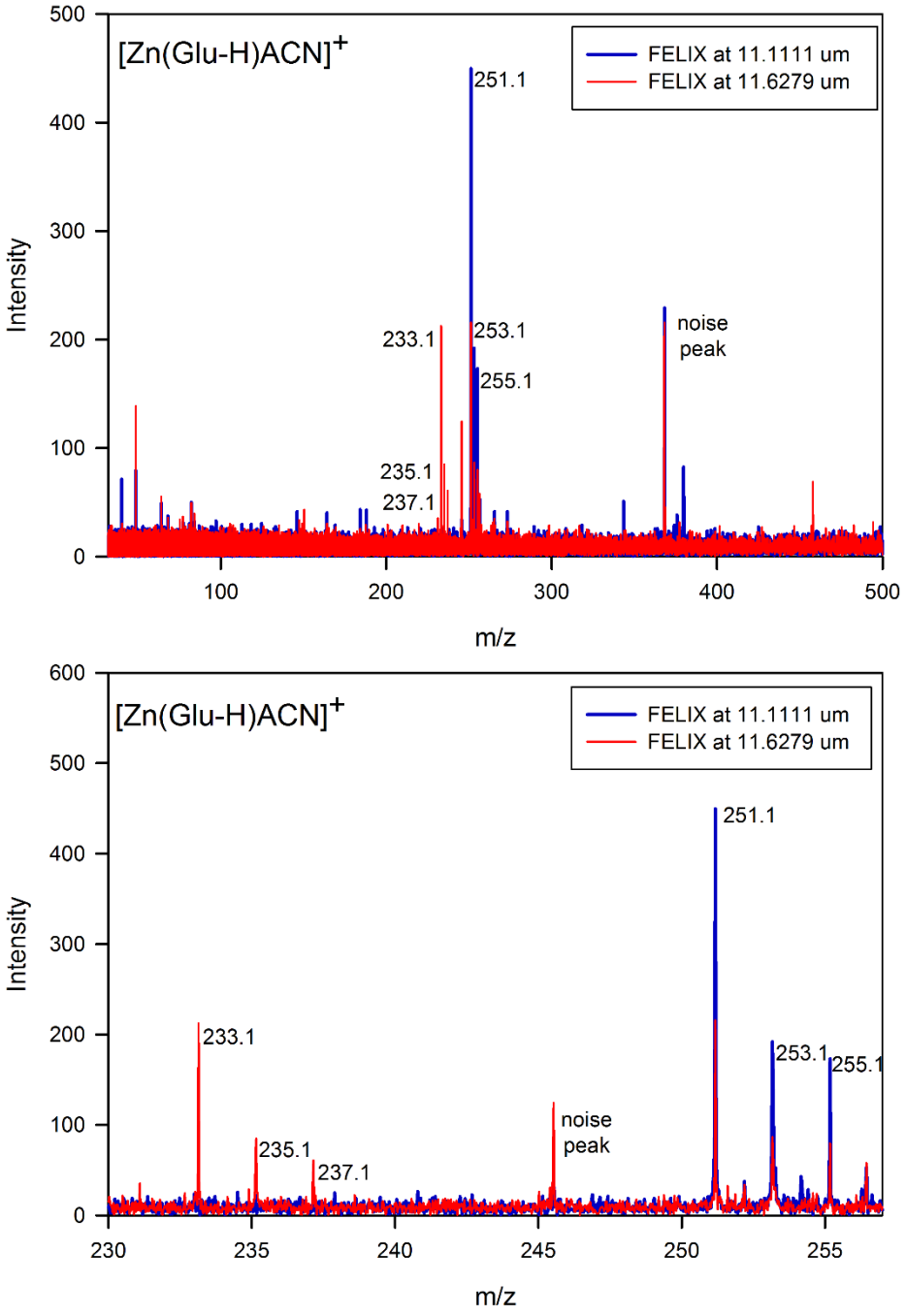

[Zn(Glu-H)ACN]+
FELIX at 11.1111 um
FELIX at 11.6279 um
251.1
233.1
253.1
255.1
noise
peak
235.1
237.1
Intensity
m/z
[Zn(Glu-H)ACN]+
FELIX at 11.1111 um
FELIX at 11.6279 um
251.1
233.1
253.1
255.1
noise
peak
235.1
237.1
Intensity
m/z

Figure S1

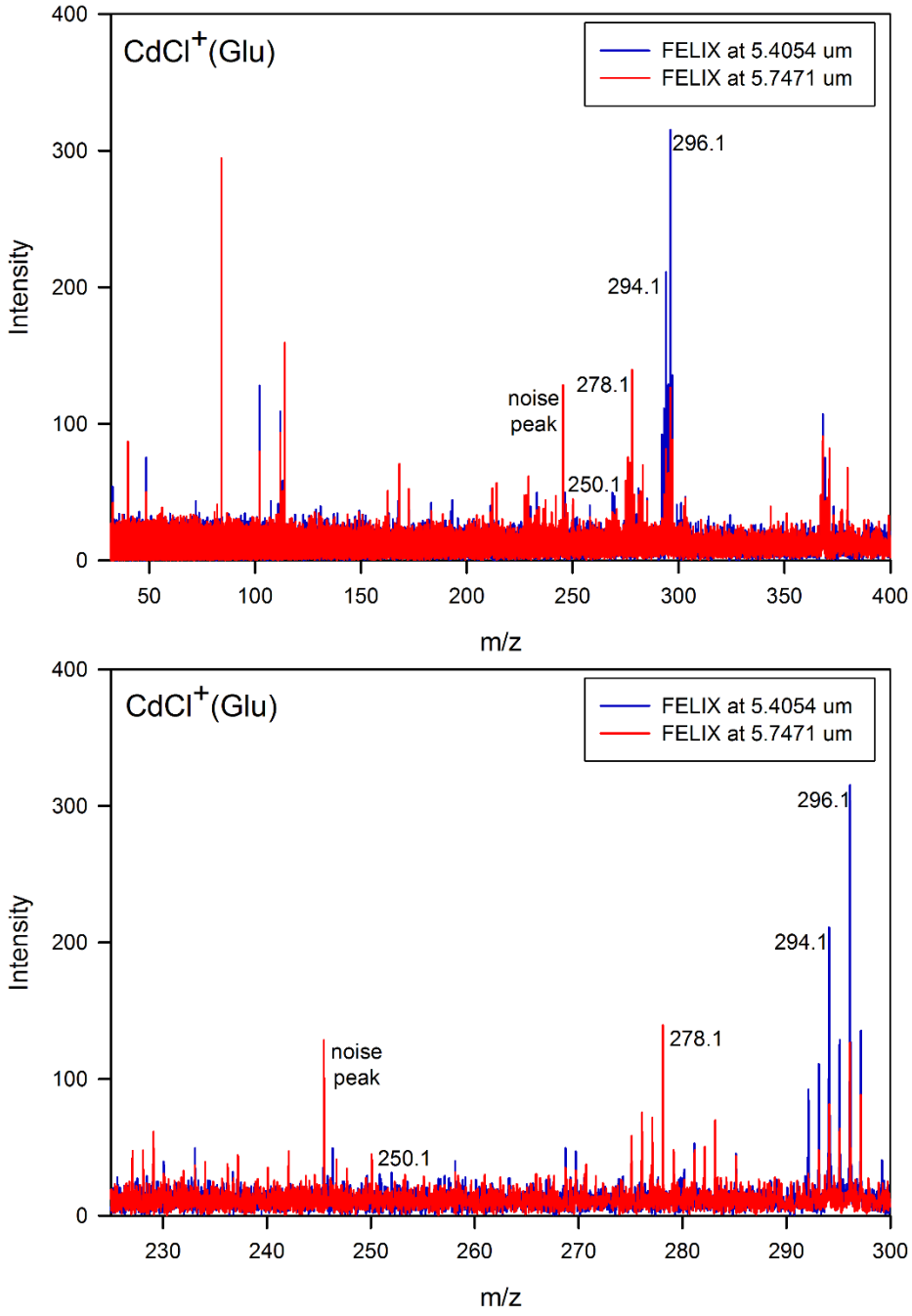
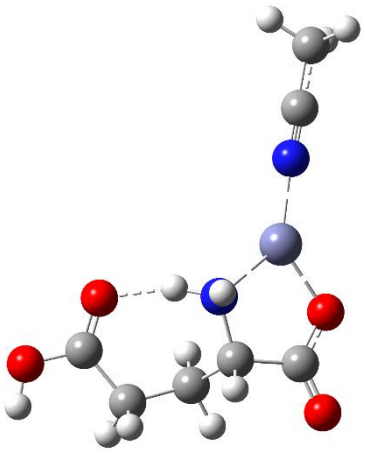
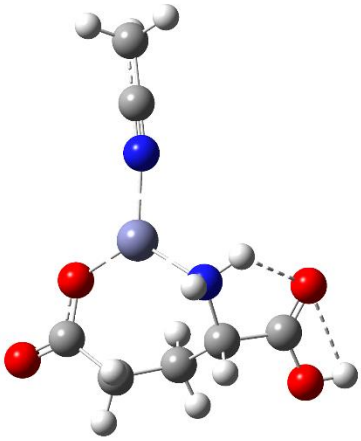

CdCl+(Glu)
FELIX at 5.4054 um
FELIX at 5.7471 um
296.1
294.1
278.1
noise
peak
250.1
Intensity
m/z
CdCl+(Glu)
FELIX at 5.4054 um
FELIX at 5.7471 um
296.1
294.1
278.1
noise
peak
250.1
Intensity
m/z

Figure S2



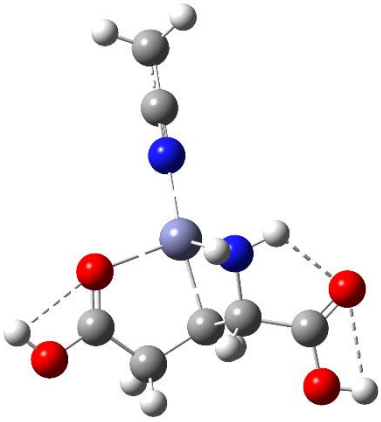
[N,CO^{-}]-gtgtc

(66.3, 69.4, 78.7)



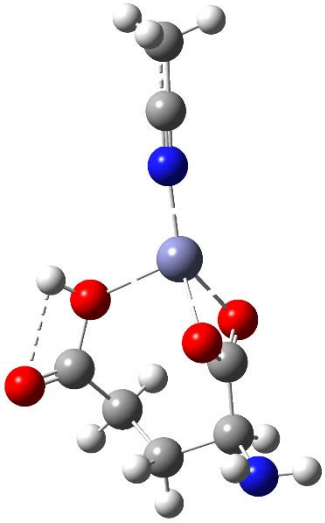
[N,CO_s^{-}]-tgtgg

(79.1, 83.0, 86.9)



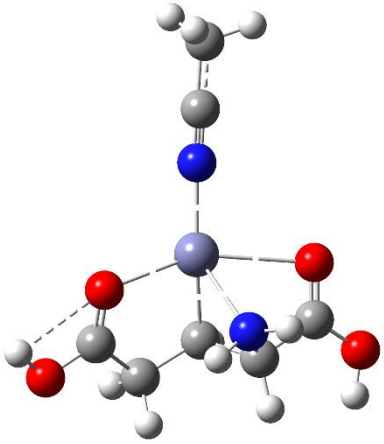
[N,C_y^{-},CO]-ttgggt

(86.7, 84.5, 91.4)



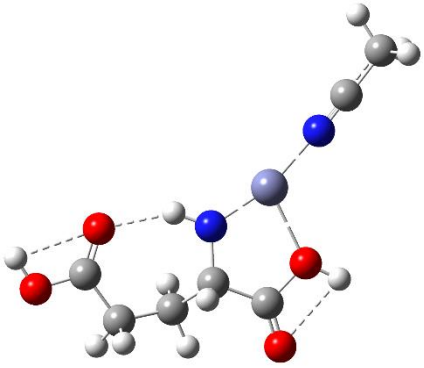
[CO_2^{-},OH_s]-gcggt

(89.5, 94.8, 91.4)



[N,C_y^{-},CO_s,CO]-cgtgtt

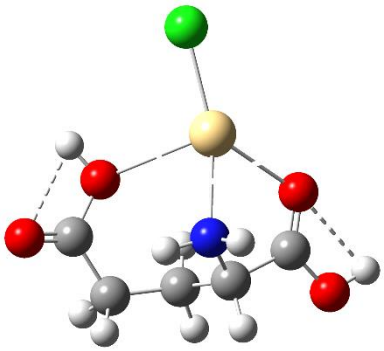
(114.7, 110.7, 110.6)



[N^{-},OH]-tttgtt

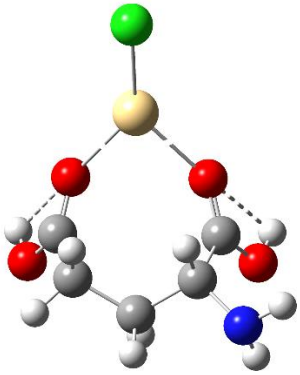
(142.5, 150.5, 152.8)

Figure S3



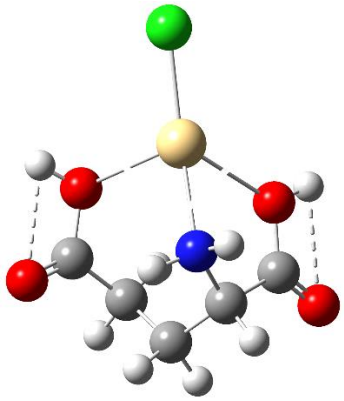
[N,CO,OH_s]-tgtgct

(49.9, 50.0, 43.3)



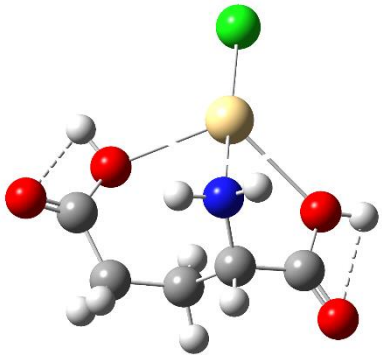
[CO_s,CO]-tggggt

(68.4, 74.1, 86.8)



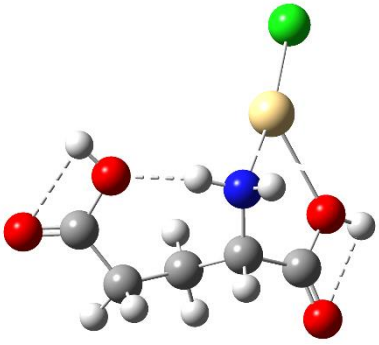
[N,OH,OH_s]-tggggt

(77.9, 81.0, 66.8)



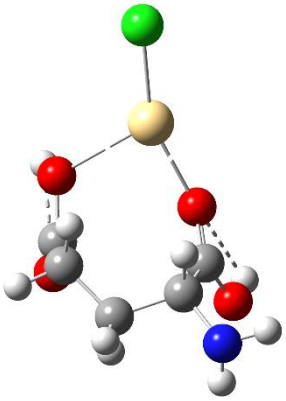
[N,OH,OH_s]-tgtgct

(83.5, 86.3, 73.2)



[N,OH]-tgtgct

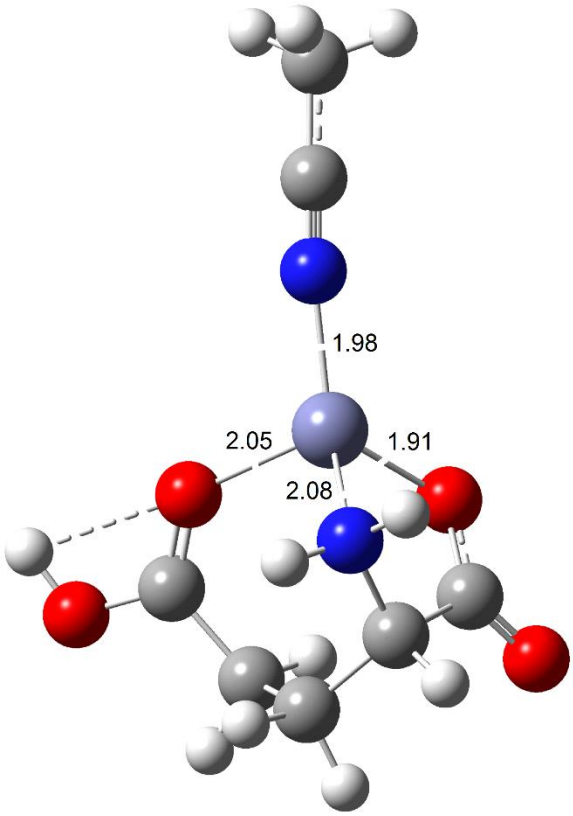
(86.5, 91.3, 88.2)



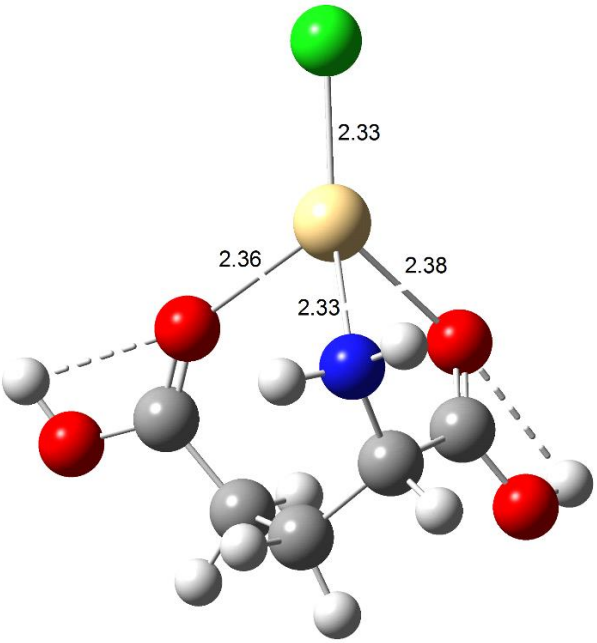
[CO,OH_s]-tggggt

(114.1, 120.6, 123.7)

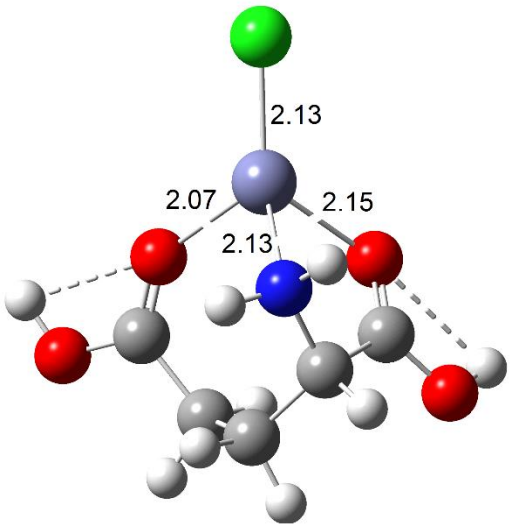
Figure S4



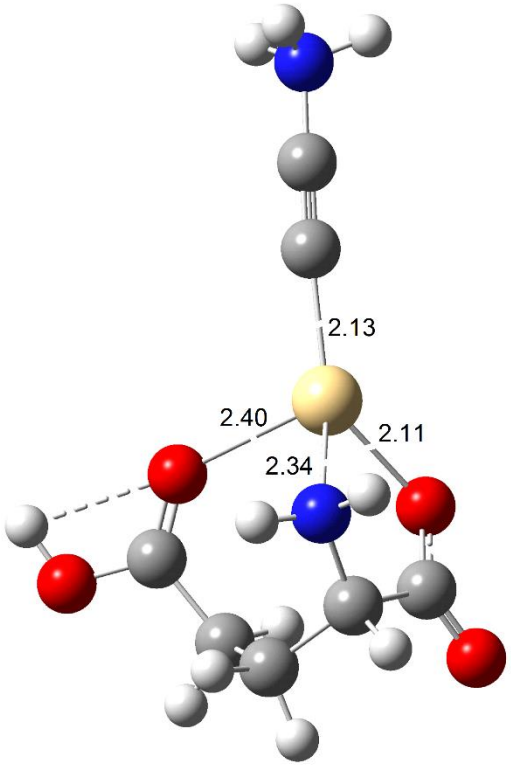
[Zn(Glu-H)ACN]$^{+}$
[N,CO^{-},CO$_s$]-gcggt



CdCl^{+}(Glu)
[N,CO$_s$,CO]-tgcggt



ZnCl^{+}(Glu)
[N,CO$_s$,CO]-tgcggt



[Cd(Glu-H)ACN]$^{+}$
[N,CO^{-},CO$_s$]-gcggt

Figure S5

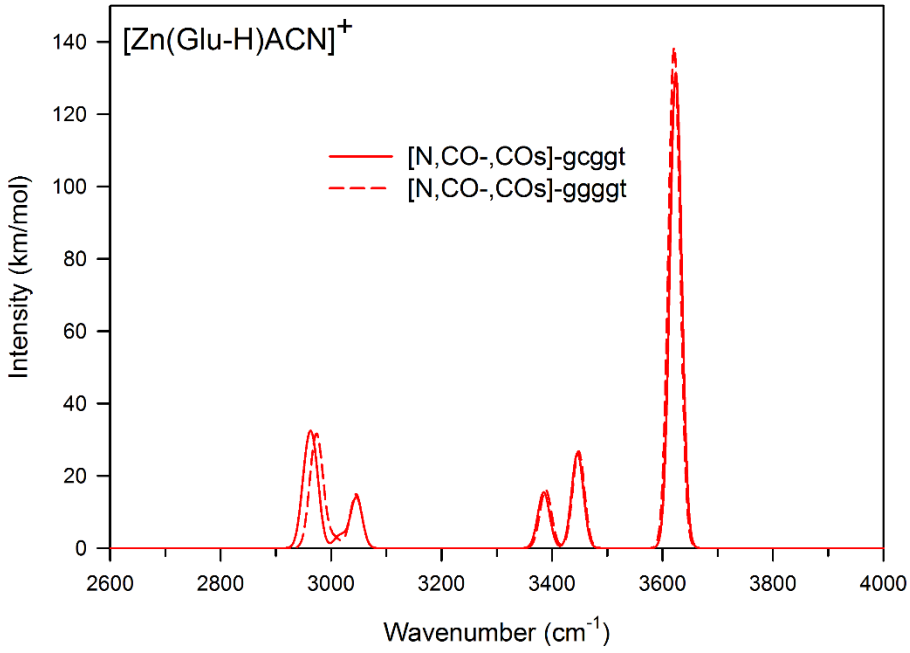


Figure S6

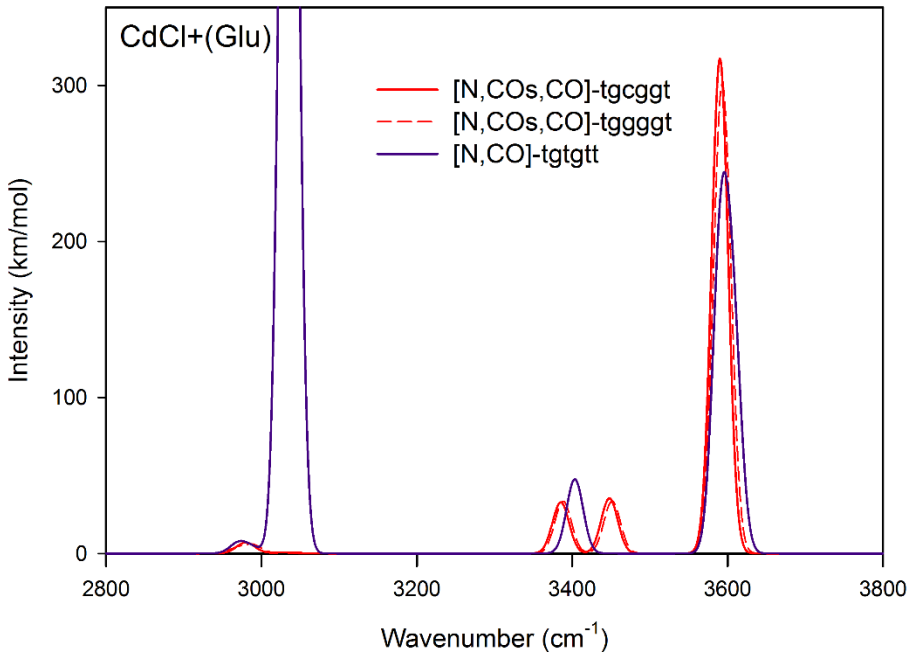


Figure S7