ARTICLE – SUPPORTING INFORMATION

Characterization of Holmium(III)-Acetylacetonate Complexes Derived from Therapeutic Microspheres by Infrared Ion Spectroscopy

Kas J. Houthuijs,[a] Jonathan Martens,*[a] Alexandra G. Arranja,[b,c,d] Giel Berden,[a] J. Frank W. Nijsen,[c,d] and Jos Oomens *[a,e]

a. Radboud University, Institute for Molecules and Materials, FELIX Laboratory, Toernooiveld 7, 6525ED Nijmegen, The Netherlands. E-mail: jonathan.martens@ru.nl, j.oomens@science.ru.nl
b. Department of Pharmaceutics, Utrecht Institute for Pharmaceutical Sciences (UIPS), Utrecht University, PO Box 80082, 3508 TB Utrecht, The Netherlands.
c. Radboudumc, Department of Radiology and Nuclear Medicine, Geert Grooteplein Zuid 10, 6525 GA Nijmegen, The Netherlands.
d. Quirem Medical B.V., Zutphenseweg 55, 7418 AH Deventer, The Netherlands.
e. van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Science Park 908, 1098 XH Amsterdam, The Netherlands.

Supporting Information
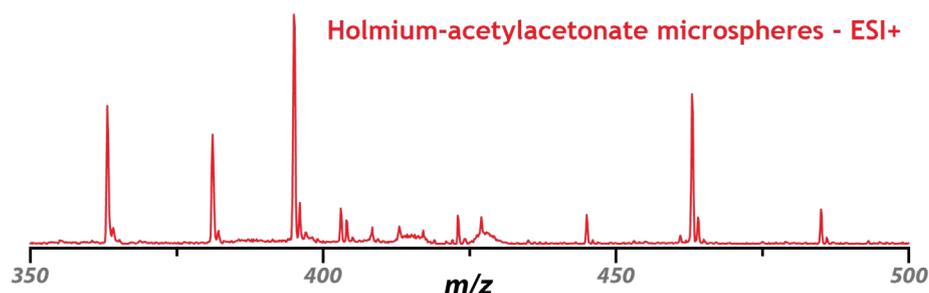
Figure S1. Mass spectrum (ESI+) of the holmium-acetylacetonate microspheres.
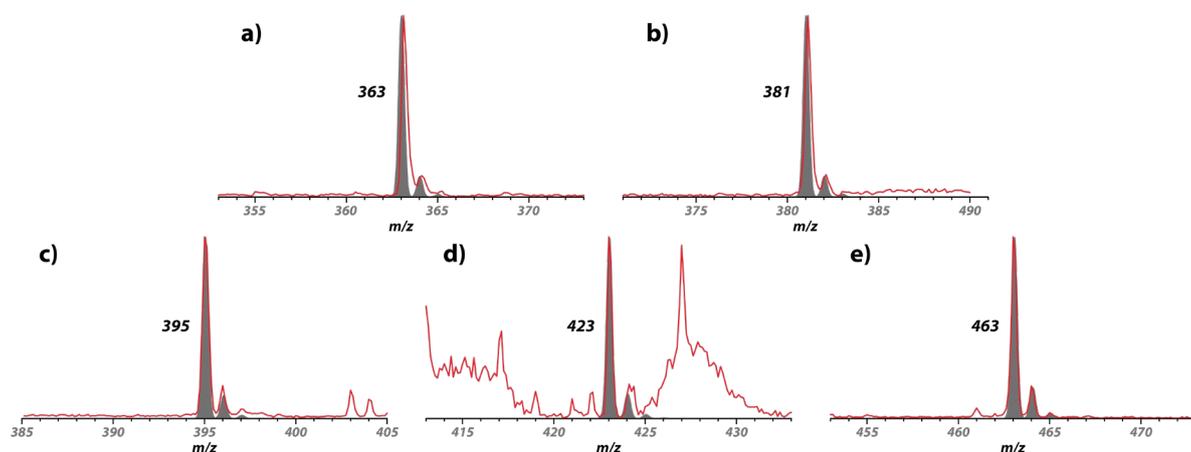

Figure S2. Mass spectra (red) of the complexes under investigation overlaid with a simulation of the isotope pattern of the assigned complexes (grey): [Ho(acac)$_2$ – 2H]$^+$ (a), [Ho(acac)$_2$(H$_2$O) – 2H]$^+$ (b), [Ho(acac)$_2$(MeOH) – 2H]$^+$ (c), [Ho(acac)$_2$(CH$_3$COOH) – 2H]$^+$ (d) and [Ho(acac)$_3$ – 2H]$^+$ (e).
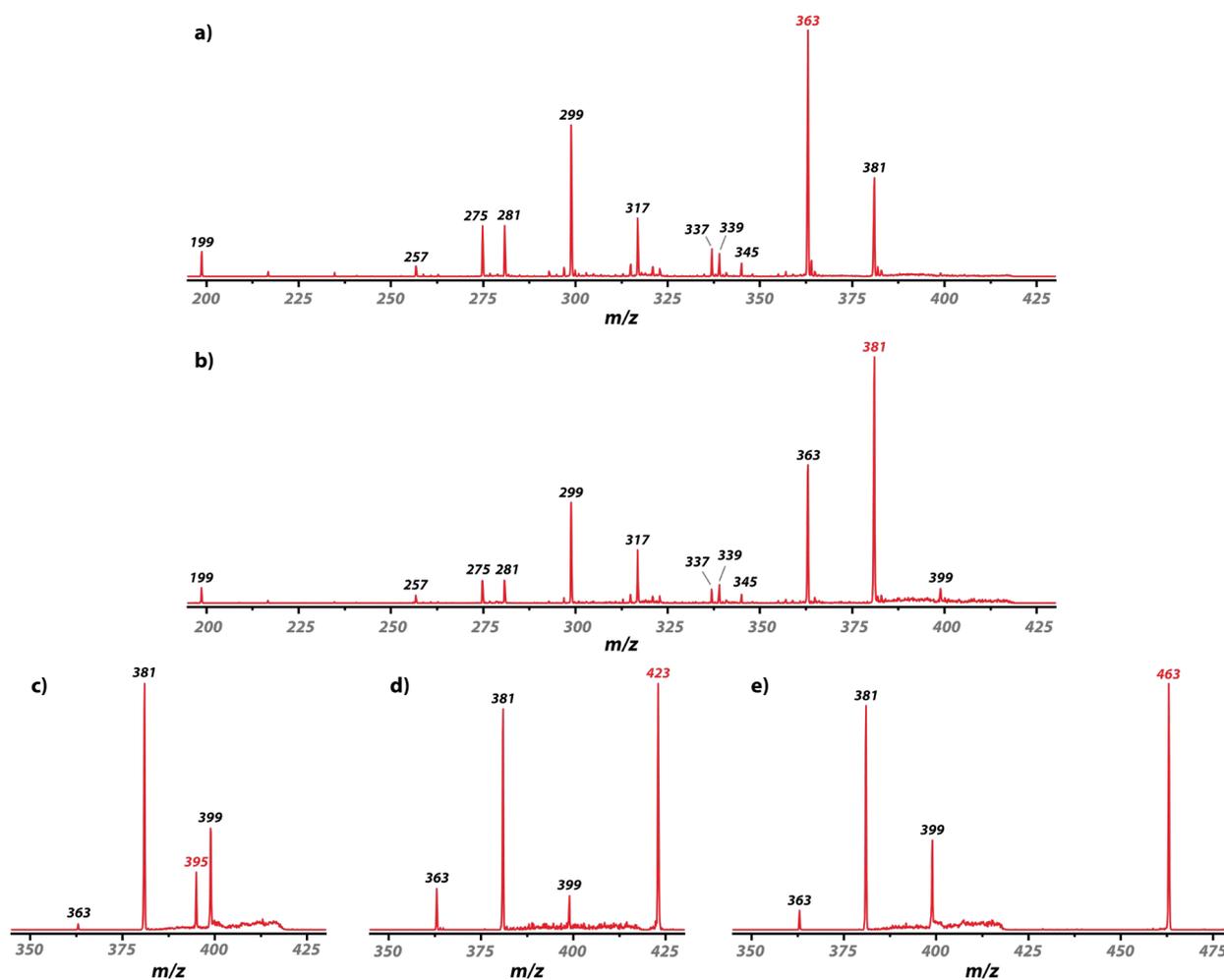
Figure S3. IRMPD fragmentation mass spectra for each of the complexes under investigation: [Ho(acac)$_2$ − 2H]$^+$ (a), [Ho(acac)$_2$(H$_2$O) − 2H]$^+$ (b), [Ho(acac)$_2$(MeOH) − 2H]$^+$ (c), [Ho(acac)$_2$(CH$_3$COOH) − 2H]$^+$ (d) and [Ho(acac)$_3$ − 2H]$^+$ (e). The precursor mass for each of the fragmentation spectra is indicated in red. The spectra were reconstructed from the strongest absorption bands for each complex.
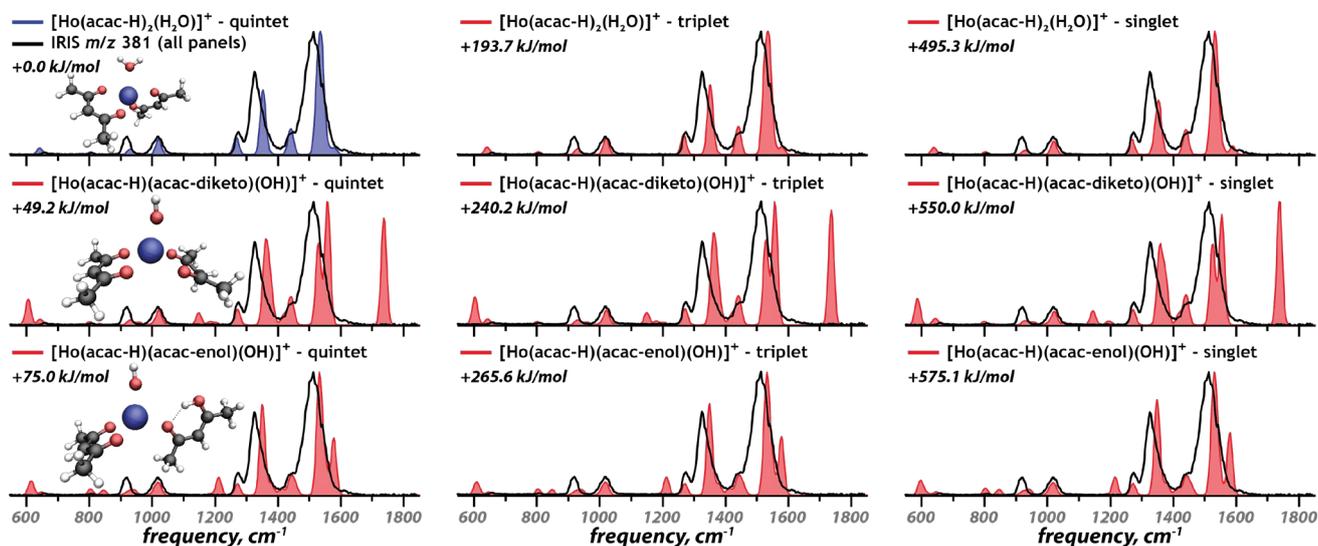
Figure S4. Comparison of the calculated spectra (coloured) of the three spin states of each considered geometry for the [Ho(acac)$_2$H$_2$O − 2H]$^+$ complex to experimental spectrum of the m/z 381 ion (black). Inscribed are the relative energies of the computed structures. The displayed geometries represent the geometries of each row.
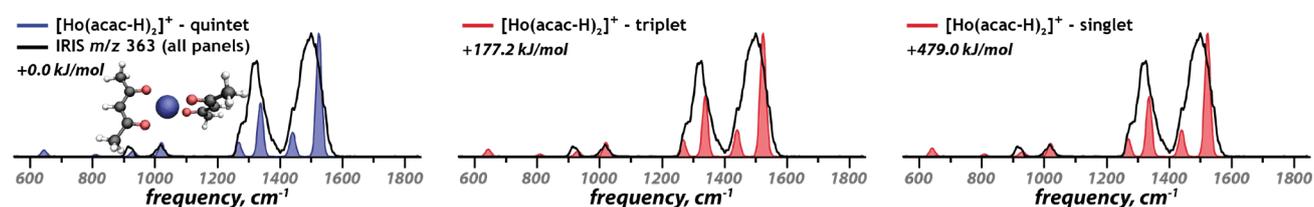
Figure S5. Comparison of the calculated spectra (coloured) of the three spin states of the [Ho(acac − H)$_2$]$^+$ complex to experimental spectrum of the m/z 363 ion (black). Inscribed are the relative energies of the computed structures. The displayed geometry represents the geometries of the entire row.
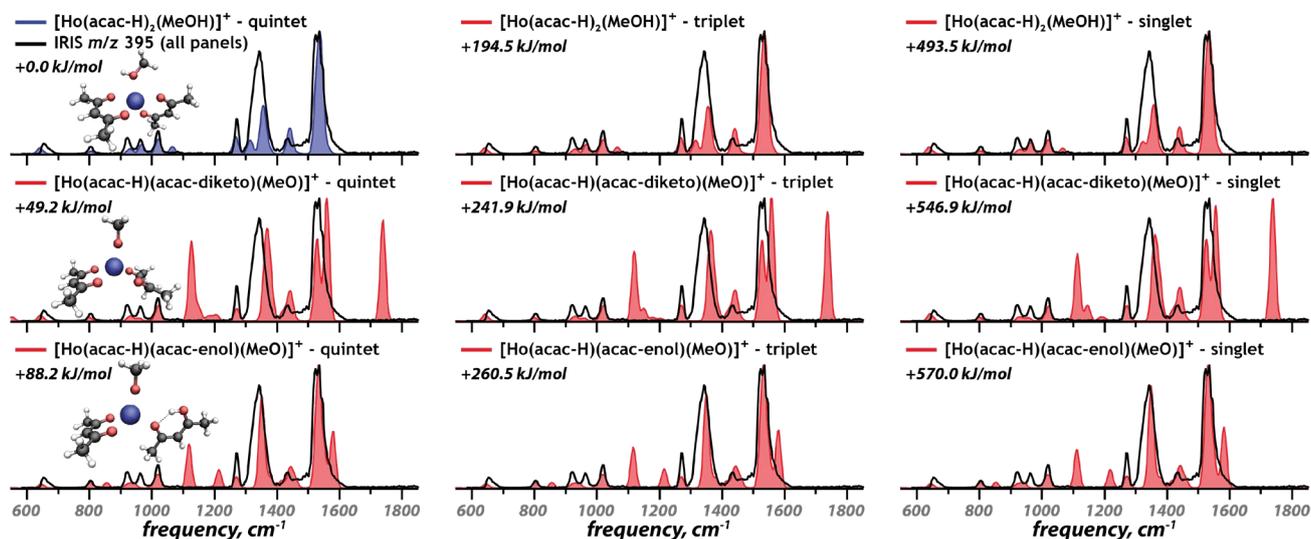
Figure S6. Comparison of the calculated spectra (coloured) of the three spin states of each considered geometry for the [Ho(acac)$_2$MeOH − 2H]$^+$ complex to experimental spectrum of the m/z 395 ion (black). Inscribed are the relative energies of the computed structures. The displayed geometries represent the geometries of each row.
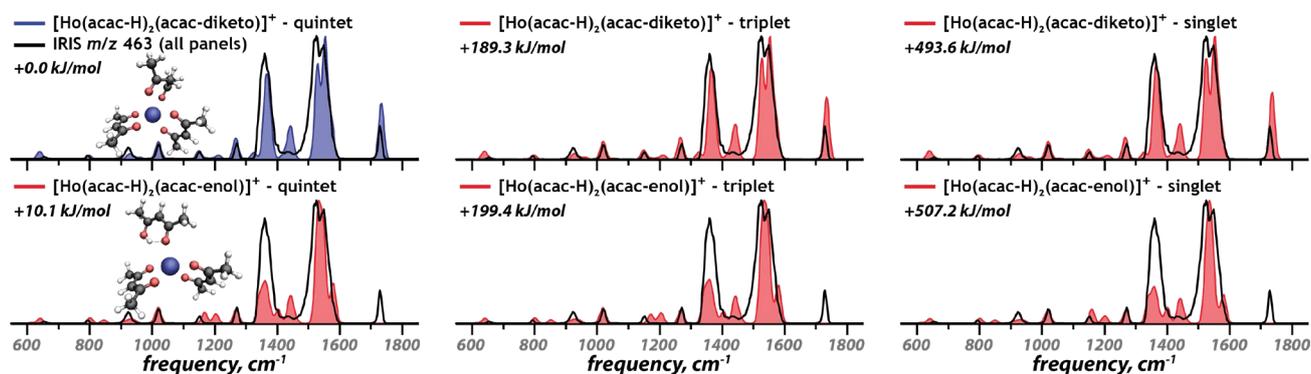
**Figure S7.** Comparison of the calculated spectra (coloured) of the three spin states of each considered geometry for the [Ho(acac)$_3$ − 2H]$^+$ complex to experimental spectrum of the m/z 463 ion (black). Inscribed are the relative energies of the computed structures. The displayed geometries represent the geometries of each row.

Table S1. Calculated harmonic frequencies, scaled frequencies (0.975) and corresponding intensities of the vibrational analysis on the assigned ionic complexes presented in Figure 2.

[Ho(acac-H)$_2$]$^+$			[Ho(acac-H)$_2$(H$_2$O)]$^+$			[Ho(acac-H)$_2$(MeOH)]$^+$			[Ho(acac-H)$_2$(acac)]$^+$		
$\nu_{harm.}$ (cm^{-1})	ν_{scaled} (cm^{-1})	Intensity (km·mol^{-1})	$\nu_{harm.}$ (cm^{-1})	ν_{scaled} (cm^{-1})	Intensity (km·mol^{-1})	$\nu_{harm.}$ (cm^{-1})	ν_{scaled} (cm^{-1})	Intensity (km·mol^{-1})	$\nu_{harm.}$ (cm^{-1})	ν_{scaled} (cm^{-1})	Intensity (km·mol^{-1})
24.0	23.4	0.2	16.5	16.1	3.2	19.6	19.1	0.5	21.2	20.7	0.2
25.3	24.7	0.3	25.2	24.6	2.0	27.6	26.9	0.8	24.8	24.2	1.3
36.0	35.1	0.0	28.9	28.2	0.8	28.8	28.0	1.0	28.0	27.3	0.5
86.5	84.4	0.0	31.8	31.0	0.2	32.2	31.4	0.3	29.1	28.4	1.6
86.6	84.4	0.0	67.8	66.1	5.2	53.3	51.9	1.4	31.7	30.9	0.1
98.4	95.9	0.0	79.1	77.1	0.5	79.3	77.3	0.4	35.8	34.9	3.4
98.6	96.1	0.0	79.6	77.6	0.6	80.2	78.2	0.7	76.3	74.4	2.0
115.8	112.9	21.3	97.6	95.1	0.0	94.4	92.0	0.8	83.9	81.8	0.4
117.6	114.7	21.7	98.0	95.6	0.0	97.4	95.0	0.0	86.5	84.3	0.9
119.5	116.5	0.0	112.6	109.8	7.2	98.5	96.1	0.1	92.8	90.5	1.5
149.8	146.1	0.0	118.5	115.6	0.3	112.7	109.9	2.9	97.7	95.3	0.1
165.2	161.1	0.3	120.7	117.7	18.3	119.4	116.4	5.2	99.1	96.6	0.0
165.3	161.1	0.3	146.3	142.7	6.3	123.7	120.6	9.1	113.3	110.5	4.7
174.5	170.2	0.0	163.5	159.4	0.0	131.2	127.9	12.8	120.2	117.2	4.3
223.1	217.5	6.6	164.4	160.3	1.2	143.8	140.3	8.0	128.9	125.7	5.2
250.9	244.7	0.0	186.2	181.5	0.3	163.1	159.0	0.1	133.4	130.1	1.8
257.5	251.0	6.0	230.5	224.8	4.0	164.3	160.1	1.5	138.0	134.5	2.1
258.4	251.9	5.8	231.9	226.1	3.7	185.0	180.4	0.9	144.8	141.1	2.1
262.3	255.8	43.0	235.4	229.5	13.1	191.7	186.9	0.3	153.4	149.5	4.9
403.4	393.4	17.1	249.7	243.4	0.4	228.1	222.4	9.2	161.3	157.3	2.8
404.2	394.1	17.0	254.4	248.0	27.9	233.9	228.1	2.0	163.7	159.6	1.0
443.8	432.7	167.6	306.2	298.6	9.8	236.0	230.1	11.8	165.9	161.7	1.1
452.1	440.8	0.2	339.4	330.9	0.2	249.4	243.1	0.5	175.1	170.7	19.5
549.7	536.0	14.1	344.8	336.2	233.4	255.0	248.6	40.6	191.0	186.2	2.1
550.5	536.7	14.1	405.4	395.3	12.2	307.0	299.3	17.0	221.8	216.2	12.1
567.9	553.7	0.0	406.3	396.1	30.7	406.8	396.6	15.7	222.8	217.2	24.9
568.2	554.0	0.0	429.0	418.2	89.0	407.8	397.6	13.2	236.6	230.7	14.3
660.0	643.5	111.7	442.7	431.6	1.2	430.6	419.9	124.9	239.9	233.9	0.4
668.8	652.1	0.0	481.7	469.6	131.7	441.1	430.0	3.5	245.3	239.2	35.0
669.2	652.5	3.2	542.2	528.6	20.4	485.1	472.9	113.5	246.6	240.5	14.2
669.3	652.6	3.1	542.8	529.2	11.3	540.9	527.4	21.0	356.9	348.0	2.7
830.2	809.4	16.0	568.0	553.8	0.1	542.0	528.4	10.7	362.2	353.1	23.5
830.9	810.2	15.8	568.2	554.0	0.0	567.9	553.7	0.0	406.7	396.6	18.9
952.3	928.5	29.4	657.2	640.7	85.2	568.4	554.2	0.1	409.1	398.9	12.1
952.5	928.7	29.2	664.1	647.5	2.4	656.8	640.4	75.6	421.2	410.6	88.3
954.3	930.5	29.9	670.3	653.5	6.0	663.4	646.8	3.9	433.8	423.0	19.9
955.0	931.1	11.2	670.7	654.0	3.2	670.3	653.6	3.7	491.8	479.5	2.7
1038.4	1012.4	4.7	825.4	804.8	14.0	671.5	654.7	5.1	511.2	498.4	0.8
1038.5	1012.5	4.6	825.7	805.0	20.1	824.8	804.2	15.7	533.7	520.3	12.6
1044.3	1018.2	18.3	951.1	927.3	31.9	825.3	804.7	18.5	535.6	522.2	44.1
1044.4	1018.3	18.1	951.7	927.9	15.4	950.8	927.0	31.6	536.7	523.3	11.3
1047.2	1021.0	213.2	957.8	933.8	31.3	951.9	928.1	15.1	569.1	554.9	0.0
1051.2	1024.9	0.1	958.2	934.2	0.5	958.3	934.3	22.2	569.3	555.1	0.1
1057.5	1031.0	0.0	1037.5	1011.6	4.6	958.7	934.7	8.1	654.4	638.0	13.2
1057.6	1031.1	0.0	1037.7	1011.7	5.8	992.0	967.2	132.0	654.6	638.3	49.5
1222.1	1191.5	0.3	1044.6	1018.5	13.1	1037.3	1011.4	6.3	660.5	644.0	9.4
1222.1	1191.6	0.3	1044.8	1018.6	18.6	1037.4	1011.4	6.6	672.0	655.2	4.1
1299.9	1267.4	260.4	1046.7	1020.5	165.8	1044.4	1018.3	15.1	672.5	655.7	4.5
1306.0	1273.3	0.2	1050.0	1023.7	8.1	1044.9	1018.7	16.3	786.9	767.2	5.1
1371.2	1336.9	499.1	1058.1	1031.7	0.1	1046.7	1020.5	157.5	817.4	797.0	17.0
1371.8	1337.5	500.2	1058.2	1031.8	0.2	1050.1	1023.8	7.6	818.2	797.8	19.0
1403.7	1368.6	0.4	1223.8	1193.2	4.4	1058.1	1031.6	0.1	849.9	828.6	4.3
1403.8	1368.7	0.4	1223.9	1193.3	0.8	1058.3	1031.9	0.1	888.9	866.6	3.5
1407.1	1371.9	0.0	1299.7	1267.2	241.0	1092.7	1065.4	99.1	948.5	924.7	25.0
1407.1	1371.9	0.0	1305.4	1272.8	3.4	1174.7	1145.4	1.1	950.4	926.7	14.3
1469.0	1432.3	0.1	1384.6	1350.0	309.4	1223.6	1193.0	2.9	959.2	935.2	10.4
1469.2	1432.5	0.3	1388.6	1353.9	612.0	1224.6	1194.0	2.2	960.0	936.0	6.0
1469.9	1433.1	22.7	1404.7	1369.6	0.0	1300.2	1267.7	229.5	966.2	942.1	9.7
1470.0	1433.2	22.5	1404.8	1369.7	0.1	1305.7	1273.1	7.3	986.2	961.5	15.7
1477.9	1441.0	412.6	1407.9	1372.7	4.5	1348.2	1314.5	185.9	1030.8	1005.0	3.3
1480.2	1443.2	0.1	1408.7	1373.5	23.1	1385.7	1351.0	348.7	1036.1	1010.2	7.4
1483.5	1446.4	1.5	1470.7	1434.0	3.7	1394.7	1359.8	400.0	1036.7	1010.8	4.6
1483.6	1446.5	1.4	1470.8	1434.0	8.4	1404.7	1369.6	0.0	1044.4	1018.3	11.2
1561.7	1522.7	1354.5	1472.4	1435.6	14.9	1405.0	1369.9	0.1	1045.1	1019.0	18.0
1566.7	1527.6	518.6	1472.6	1435.7	15.2	1407.9	1372.7	5.0	1045.9	1019.8	101.0
1566.9	1527.7	520.2	1478.8	1441.8	307.9	1410.3	1375.0	56.0	1048.8	1022.6	29.6

1586.6	1547.0	1.4
3052.0	2975.7	1.6
3052.1	2975.8	0.2
3052.1	2975.8	0.2
3052.1	2975.8	0.3
3111.2	3033.4	0.0
3111.2	3033.4	0.0
3111.2	3033.4	0.8
3111.2	3033.5	0.7
3167.0	3087.8	23.9
3167.1	3088.0	6.6
3167.2	3088.0	1.0
3167.3	3088.2	1.0
3235.9	3155.0	0.1
3235.9	3155.0	0.0

1480.6	1443.6	21.0
1485.7	1448.5	1.1
1485.7	1448.6	1.7
1565.7	1526.5	688.0
1567.4	1528.2	386.8
1580.1	1540.6	1271.3
1600.2	1560.2	85.4
1620.9	1580.4	89.5
3052.0	2975.7	0.5
3052.1	2975.8	0.6
3052.1	2975.8	0.3
3052.2	2975.9	0.2
3111.6	3033.8	1.3
3111.6	3033.8	1.3
3111.8	3034.0	1.4
3111.8	3034.0	1.3
3163.2	3084.1	22.7
3163.2	3084.1	1.7
3163.8	3084.7	8.8
3163.8	3084.7	3.1
3234.2	3153.4	0.7
3234.3	3153.4	0.4
3783.2	3688.6	97.6
3887.0	3789.8	165.3

1470.9	1434.1	3.8
1471.0	1434.2	8.4
1472.3	1435.5	16.4
1473.3	1436.5	15.5
1478.8	1441.8	282.6
1480.4	1443.4	24.6
1481.1	1444.0	12.0
1486.1	1448.9	1.3
1486.8	1449.7	0.7
1501.2	1463.7	8.6
1508.1	1470.4	6.8
1566.6	1527.4	611.6
1568.4	1529.2	388.9
1581.1	1541.6	1274.7
1602.6	1562.6	78.3
3051.5	2975.2	0.9
3052.1	2975.8	0.4
3052.1	2975.8	0.4
3052.2	2975.9	0.2
3074.6	2997.7	25.6
3111.1	3033.4	1.9
3111.6	3033.8	1.4
3111.8	3034.0	1.5
3112.0	3034.2	1.2
3162.5	3083.4	13.0
3162.9	3083.8	11.6
3163.1	3084.1	8.0
3163.3	3084.2	7.2
3163.3	3084.3	3.7
3192.3	3112.5	2.1
3233.8	3152.9	0.8
3233.8	3153.0	0.5
3791.1	3696.3	101.9

1058.2	1031.8	0.3
1059.1	1032.6	0.1
1081.4	1054.4	8.3
1178.8	1149.3	81.3
1204.4	1174.3	9.3
1224.5	1193.9	5.6
1225.9	1195.2	4.2
1243.7	1212.6	35.4
1298.7	1266.2	158.3
1303.6	1271.0	48.7
1358.5	1324.6	62.7
1397.0	1362.0	262.1
1398.3	1363.4	161.2
1400.5	1365.5	156.2
1401.7	1366.7	129.3
1404.6	1369.5	0.4
1404.7	1369.6	1.2
1409.4	1374.1	47.8
1412.7	1377.4	287.5
1441.7	1405.7	8.0
1457.1	1420.7	0.3
1459.0	1422.5	43.0
1467.2	1430.5	5.1
1467.8	1431.1	23.2
1472.5	1435.7	7.2
1472.9	1436.0	1.5
1473.6	1436.8	18.3
1476.0	1439.1	13.9
1480.2	1443.2	217.1
1481.5	1444.5	52.5
1488.6	1451.3	2.2
1489.7	1452.4	5.7
1567.4	1528.2	247.1
1568.0	1528.8	651.0
1593.2	1553.4	1144.9
1614.1	1573.8	357.3
1712.8	1670.0	1.1
1777.7	1733.3	536.3
3009.8	2934.6	30.5
3042.0	2965.9	5.7
3042.5	2966.4	2.9
3048.3	2972.1	5.1
3051.6	2975.3	1.8
3051.7	2975.4	1.3
3052.3	2975.9	0.8
3099.9	3022.4	0.0
3100.5	3022.9	0.0
3107.8	3030.1	5.3
3112.1	3034.3	0.1
3112.2	3034.4	5.0
3112.9	3035.1	1.9
3141.4	3062.9	2.1
3157.1	3078.2	12.9
3158.0	3079.0	18.6
3158.3	3079.3	5.5
3158.9	3079.9	9.5
3177.6	3098.1	2.0
3177.7	3098.3	1.1
3230.1	3149.3	2.2
3230.4	3149.7	2.1

ARTICLE

Table S2. Calculated harmonic frequencies, scaled frequencies (0.975) and corresponding intensities of the vibrational analysis on the ionic complexes presented in Figure 4.

[Ho(acac-H)$_2$(CH$_3$COOH-bonded)]$^+$			[Ho(acac-H)$_2$(CH$_3$COOH-cis)]$^+$			[Ho(acac-H)(acac-diketo)(CH$_3$COO)]$^+$			[Ho(acac-H)$_2$(CH$_3$COOH-trans)]$^+$			[Ho(acac-H)(acac-enol)(CH$_3$COO)]$^+$		
$\nu_{harm.}$ (cm^{-1})	ν_{scaled} (cm^{-1})	Intensity (km·mol^{-1})	$\nu_{harm.}$ (cm^{-1})	ν_{scaled} (cm^{-1})	Intensity (km·mol^{-1})	$\nu_{harm.}$ (cm^{-1})	ν_{scaled} (cm^{-1})	Intensity (km·mol^{-1})	$\nu_{harm.}$ (cm^{-1})	ν_{scaled} (cm^{-1})	Intensity (km·mol^{-1})	$\nu_{harm.}$ (cm^{-1})	ν_{scaled} (cm^{-1})	Intensity (km·mol^{-1})
23.1	22.5	0.1	14.8	14.4	1.7	21.3	20.8	0.0	18.7	18.3	0.4	8.3	8.1	0.2
25.6	24.9	0.4	18.7	18.2	2.9	25.4	24.8	2.2	20.5	19.9	0.6	13.4	13.1	0.4
27.9	27.2	0.5	22.9	22.3	0.5	32.9	32.1	1.1	23.9	23.3	0.9	23.7	23.1	1.4
31.0	30.2	0.3	26.7	26.0	2.7	34.9	34.1	0.1	26.0	25.4	0.1	24.8	24.1	0.4
34.1	33.3	0.5	28.3	27.6	0.5	42.8	41.8	0.7	28.2	27.5	0.4	33.2	32.3	0.5
64.8	63.1	1.2	29.7	28.9	1.1	49.4	48.2	2.0	30.9	30.2	0.2	33.8	33.0	0.1
84.1	82.0	1.2	39.8	38.8	0.1	65.2	63.5	1.0	80.5	78.4	0.1	48.2	47.0	1.5
84.7	82.6	0.8	57.8	56.3	1.6	86.9	84.7	0.3	81.1	79.1	0.1	68.6	66.9	0.2
89.2	87.0	0.3	83.7	81.6	0.3	88.9	86.7	1.7	83.3	81.3	2.9	76.9	74.9	1.3
101.0	98.5	0.0	84.6	82.5	0.8	96.9	94.5	3.0	94.2	91.8	1.4	83.5	81.4	2.9
102.9	100.3	0.6	98.9	96.4	0.2	99.4	96.9	0.0	97.0	94.5	0.1	86.4	84.3	0.5
106.5	103.9	1.8	99.4	96.9	0.1	117.1	114.2	5.4	99.5	97.0	0.2	87.1	84.9	0.4
125.9	122.7	6.3	109.7	106.9	7.4	124.9	121.7	4.6	101.7	99.2	1.0	98.7	96.2	0.0
131.0	127.7	4.7	121.5	118.4	2.6	131.3	128.0	6.2	123.7	120.6	4.7	111.9	109.1	5.1
147.8	144.1	6.6	124.6	121.5	7.2	134.1	130.8	4.6	127.4	124.2	5.5	123.2	120.1	8.5
159.2	155.2	5.3	142.3	138.7	8.4	142.9	139.4	5.1	139.8	136.3	3.5	134.8	131.4	2.7
164.7	160.6	0.4	143.7	140.1	9.8	151.1	147.3	2.8	145.5	141.9	10.7	151.7	147.9	0.3
171.0	166.7	5.9	163.2	159.1	0.5	164.4	160.3	0.4	163.0	158.9	0.2	162.3	158.3	1.4
176.9	172.5	14.4	163.8	159.7	1.2	176.3	171.9	1.3	164.0	159.9	1.6	170.0	165.8	13.8
186.1	181.5	2.3	188.7	183.9	6.5	187.4	182.8	20.5	192.3	187.5	3.8	188.2	183.5	1.3
209.4	204.2	1.8	204.1	199.0	5.7	205.7	200.6	3.2	202.5	197.5	6.1	221.3	215.8	3.9
232.6	226.7	6.2	229.4	223.6	23.7	228.2	222.5	18.0	230.8	225.1	15.8	230.7	225.0	1.7
238.9	233.0	22.5	229.7	224.0	15.4	235.7	229.8	29.3	233.1	227.3	24.9	234.5	228.7	10.5
246.8	240.6	18.9	240.3	234.3	13.0	240.3	234.3	4.6	238.7	232.7	9.7	244.2	238.1	32.1
249.6	243.3	7.0	249.5	243.2	22.8	248.2	242.0	4.8	249.4	243.2	1.4	249.5	243.3	9.6
269.2	262.4	53.3	249.8	243.6	26.6	287.2	280.0	68.4	252.0	245.7	46.2	293.9	286.6	67.2
406.9	396.7	19.0	407.1	396.9	23.2	359.0	350.0	2.8	407.9	397.7	23.0	364.5	355.4	6.5
411.3	401.0	30.9	409.3	399.1	4.7	367.1	357.9	30.1	408.9	398.7	5.4	407.8	397.6	15.2
430.5	419.7	45.6	429.4	418.7	112.1	408.8	398.6	14.5	429.3	418.6	110.2	440.7	429.7	76.3
442.5	431.4	37.8	440.8	429.8	11.5	438.3	427.3	61.4	440.8	429.8	12.4	451.0	439.7	30.6
486.6	474.4	58.7	460.7	449.2	16.2	474.5	462.7	2.2	448.0	436.8	14.1	477.3	465.3	0.4
541.3	527.8	31.2	537.4	523.9	22.5	490.1	477.8	3.0	538.6	525.1	7.5	505.6	493.0	48.4
541.7	528.1	18.3	537.8	524.4	6.5	513.7	500.8	0.7	539.0	525.5	23.3	539.9	526.4	14.0
568.1	553.9	0.0	543.0	529.4	92.0	537.3	523.9	33.9	557.5	543.6	17.5	560.5	546.4	0.9
568.9	554.7	3.3	567.8	553.6	0.1	539.0	525.5	18.1	568.2	554.0	0.1	568.6	554.4	0.2
594.9	580.0	1.3	568.0	553.8	0.0	568.0	553.8	0.0	568.3	554.1	0.1	612.6	597.2	7.4
630.7	614.9	13.9	606.4	591.2	18.6	614.4	599.1	6.0	595.7	580.8	60.1	627.8	612.1	7.2
657.7	641.3	46.6	627.0	611.3	22.3	656.7	640.3	18.6	656.4	640.0	62.4	650.2	634.0	0.7
664.0	647.4	13.4	656.5	640.1	64.7	660.8	644.3	44.9	662.7	646.2	7.5	661.0	644.5	48.3
670.2	653.5	3.6	662.7	646.2	7.0	671.5	654.7	4.7	671.1	654.3	4.0	671.3	654.5	6.6
671.8	655.0	4.5	671.4	654.6	3.8	695.8	678.4	91.1	671.4	654.6	4.0	703.2	685.6	100.2
823.7	803.1	17.0	671.5	654.7	4.8	785.0	765.4	5.3	711.0	693.2	123.3	823.2	802.6	54.2
829.2	808.5	16.3	820.2	799.7	12.6	822.2	801.7	17.8	821.8	801.2	15.5	825.9	805.3	17.7
930.0	906.7	1.5	820.5	800.0	23.5	854.9	833.5	3.3	822.3	801.7	20.1	854.6	833.2	38.7
951.2	927.4	41.0	911.7	888.9	10.3	886.1	864.0	3.7	905.3	882.6	24.4	938.2	914.8	17.7
952.7	928.9	16.0	950.5	926.8	36.0	945.3	921.7	8.4	950.6	926.9	33.1	943.7	920.1	6.0
960.2	936.2	19.9	951.8	928.0	4.7	951.9	928.1	22.3	951.9	928.1	7.5	952.2	928.4	22.5
960.9	936.9	7.8	960.6	936.6	18.8	961.2	937.1	10.1	959.9	935.9	22.0	960.6	936.6	13.3
1029.0	1003.3	62.4	961.3	937.3	2.2	968.1	943.9	6.0	960.6	936.6	2.2	970.6	946.3	43.8
1037.4	1011.5	4.3	1018.5	993.1	1.5	987.2	962.5	17.6	1036.6	1010.7	1.5	1026.9	1001.3	10.8
1039.2	1013.2	10.9	1036.5	1010.6	2.4	1026.4	1000.7	10.6	1037.2	1011.3	7.8	1035.5	1009.6	47.8
1044.3	1018.2	12.2	1037.1	1011.2	6.9	1030.1	1004.3	11.2	1039.3	1013.3	38.5	1037.0	1011.1	6.4
1044.9	1018.8	20.6	1044.8	1018.7	6.0	1037.0	1011.1	5.1	1044.7	1018.6	5.4	1040.4	1014.4	8.7
1046.2	1020.1	85.9	1045.1	1019.0	22.1	1045.2	1019.1	16.3	1045.0	1018.9	22.2	1044.8	1018.7	16.2
1048.7	1022.5	103.1	1047.0	1020.9	135.9	1049.4	1023.1	79.6	1046.7	1020.6	138.1	1045.2	1019.1	16.3
1050.6	1024.4	22.8	1050.6	1024.3	19.1	1058.8	1032.3	0.1	1050.2	1024.0	18.0	1049.5	1023.2	78.7
1058.7	1032.2	0.1	1058.6	1032.1	0.2	1071.3	1044.5	6.8	1058.5	1032.0	0.1	1058.4	1031.9	0.4
1059.5	1033.0	6.9	1058.7	1032.3	0.1	1081.8	1054.7	10.6	1058.6	1032.2	0.1	1059.1	1032.6	0.3

|														
1071.8	1045.0	6.4	1069.0	1042.3	7.5	1185.8	1156.2	90.5	1071.3	1044.5	11.5	1071.4	1044.6	10.5
1222.0	1191.5	3.4	1221.5	1191.0	117.0	1207.6	1177.5	2.0	1222.8	1192.3	2.1	1206.5	1176.3	74.1
1224.8	1194.2	2.8	1222.7	1192.1	2.7	1222.6	1192.1	3.0	1224.0	1193.4	8.5	1221.7	1191.2	3.5
1300.4	1267.9	176.4	1223.2	1192.6	10.6	1245.1	1214.0	28.7	1230.6	1199.8	119.2	1236.4	1205.5	151.4
1306.6	1274.0	73.0	1301.5	1269.0	200.8	1305.6	1272.9	115.2	1301.1	1268.5	201.1	1306.1	1273.4	129.5
1379.8	1345.3	220.6	1306.8	1274.2	17.4	1366.2	1332.0	39.0	1306.3	1273.6	21.3	1381.6	1347.1	347.4
1383.6	1349.0	131.7	1370.8	1336.5	184.5	1388.2	1353.5	24.0	1386.3	1351.6	164.0	1385.7	1351.1	321.5
1391.2	1356.4	516.5	1388.5	1353.8	120.0	1389.2	1354.4	400.2	1391.1	1356.3	189.8	1390.0	1355.2	124.2
1404.7	1369.6	0.6	1397.0	1362.1	527.3	1397.9	1363.0	90.9	1397.4	1362.4	348.0	1403.2	1368.1	48.5
1405.6	1370.5	7.8	1404.7	1369.5	0.8	1403.1	1368.1	129.3	1404.8	1369.6	1.5	1405.0	1369.9	5.3
1407.7	1372.5	5.1	1405.0	1369.9	3.4	1404.8	1369.7	0.3	1405.1	1370.0	1.5	1407.7	1372.5	5.3
1409.9	1374.7	15.3	1407.3	1372.1	2.0	1407.6	1372.5	19.6	1407.4	1372.3	0.7	1416.4	1381.0	83.4
1413.2	1377.9	118.1	1411.5	1376.3	158.6	1432.6	1396.8	87.9	1411.3	1376.1	115.3	1435.5	1399.6	47.3
1453.4	1417.1	107.1	1424.4	1388.8	171.0	1451.4	1415.1	113.2	1444.4	1408.3	160.4	1447.3	1411.2	155.0
1470.6	1433.8	9.1	1466.8	1430.1	21.9	1456.6	1420.2	0.1	1468.8	1432.1	50.5	1463.3	1426.8	212.6
1471.2	1434.4	0.0	1471.9	1435.1	2.9	1457.8	1421.4	42.4	1471.6	1434.8	2.0	1467.4	1430.8	12.1
1472.0	1435.2	20.7	1472.0	1435.2	5.0	1466.5	1429.8	9.0	1471.7	1434.9	9.2	1470.7	1433.9	4.0
1474.5	1437.6	14.2	1473.1	1436.2	9.1	1467.0	1430.3	20.1	1472.7	1435.9	17.1	1471.8	1435.0	19.9
1476.9	1440.0	51.8	1473.1	1436.3	22.6	1470.3	1433.5	108.8	1474.0	1437.1	13.1	1474.6	1437.8	23.0
1479.0	1442.0	222.9	1479.4	1442.4	6.9	1471.7	1434.9	0.6	1479.3	1442.4	249.1	1480.0	1443.0	157.3
1480.7	1443.7	68.7	1479.7	1442.7	259.1	1472.4	1435.6	24.0	1481.1	1444.1	45.1	1483.8	1446.7	10.4
1485.8	1448.7	5.2	1481.5	1444.4	39.8	1480.7	1443.7	170.7	1486.6	1449.5	3.5	1486.0	1448.9	13.4
1488.0	1450.8	9.3	1486.9	1449.7	2.0	1486.3	1449.1	0.1	1487.3	1450.2	3.0	1490.7	1453.4	120.1
1528.5	1490.3	163.9	1487.4	1450.2	1.7	1493.2	1455.9	298.6	1489.3	1452.1	51.2	1498.5	1461.1	211.7
1565.2	1526.1	348.0	1567.2	1528.0	771.3	1544.8	1506.2	230.1	1565.6	1526.4	525.0	1531.5	1493.2	217.0
1569.8	1530.5	683.8	1567.3	1528.2	191.5	1569.4	1530.2	495.0	1568.6	1529.4	453.2	1568.6	1529.4	534.7
1586.8	1547.2	828.7	1589.4	1549.7	1226.9	1595.2	1555.3	747.9	1587.5	1547.8	1181.1	1574.4	1535.0	780.8
1603.5	1563.4	484.1	1610.8	1570.6	243.0	1700.8	1658.3	1.5	1607.2	1567.0	302.6	1594.2	1554.3	295.4
1674.4	1632.6	570.7	1763.1	1719.0	673.7	1768.5	1724.3	589.1	1712.3	1669.5	737.0	1615.7	1575.3	613.5
2963.6	2889.5	1852.3	3052.1	2975.8	0.6	2999.7	2924.7	35.2	3051.4	2975.1	1.6	3048.0	2971.8	1.3
3047.4	2971.2	0.1	3052.1	2975.8	0.0	3041.9	2965.8	7.9	3051.9	2975.6	0.6	3052.2	2975.9	0.4
3052.0	2975.7	0.5	3052.1	2975.8	1.6	3042.2	2966.2	3.8	3052.5	2976.1	0.4	3052.4	2976.1	0.2
3052.6	2976.3	0.1	3052.1	2975.8	1.1	3052.0	2975.7	0.2	3052.6	2976.2	0.5	3055.4	2979.0	3.7
3052.9	2976.6	0.2	3055.9	2979.5	3.3	3052.1	2975.8	0.8	3060.5	2984.0	3.4	3060.8	2984.3	1.0
3061.6	2985.1	0.8	3112.2	3034.4	1.5	3063.4	2986.8	0.3	3111.5	3033.7	2.6	3109.2	3031.4	0.6
3107.1	3029.4	1.2	3112.2	3034.4	1.5	3100.0	3022.5	0.1	3111.7	3033.9	1.7	3112.1	3034.3	0.7
3111.7	3033.9	1.4	3112.6	3034.8	2.4	3100.1	3022.6	0.0	3112.6	3034.8	1.6	3112.2	3034.4	1.9
3112.9	3035.1	1.1	3112.6	3034.8	2.8	3112.3	3034.5	0.9	3113.1	3035.2	1.8	3114.9	3037.0	0.1
3113.0	3035.2	0.7	3120.2	3042.2	0.3	3112.4	3034.6	2.4	3136.6	3058.2	1.8	3134.7	3056.3	1.8
3140.1	3061.6	0.7	3159.8	3080.9	19.7	3130.9	3052.6	1.0	3160.6	3081.6	12.7	3163.0	3083.9	12.9
3162.7	3083.6	15.2	3160.0	3081.0	10.3	3139.9	3061.4	2.0	3161.2	3082.2	18.2	3163.4	3084.3	6.1
3163.0	3083.9	4.7	3160.3	3081.3	6.5	3161.0	3082.0	14.9	3161.4	3082.4	2.1	3165.6	3086.5	4.9
3163.5	3084.4	6.8	3160.4	3081.4	5.9	3161.4	3082.4	6.2	3161.6	3082.5	6.9	3175.1	3095.8	4.7
3164.3	3085.2	6.8	3188.3	3108.6	0.4	3176.9	3097.5	4.2	3184.3	3104.7	1.9	3179.9	3100.4	1.0
3188.2	3108.5	0.1	3232.6	3151.8	1.4	3178.3	3098.8	1.5	3233.4	3152.5	1.1	3234.7	3153.8	0.5
3234.7	3153.9	0.6	3232.7	3151.9	1.1	3178.7	3099.2	1.5	3233.5	3152.7	0.8	3245.9	3164.7	0.4
3235.0	3154.2	0.3	3774.2	3679.8	150.8	3233.7	3152.8	1.0	3722.9	3629.9	107.9	3494.3	3406.9	253.8

Atom coordinates of all presented structures with 5 spin multiplicity, as presented in Figures 1, 2, 4, S4, S5, S6 and S7.

m/z 363, [Ho(acac-H)2]+, +0.0 kJ/mol
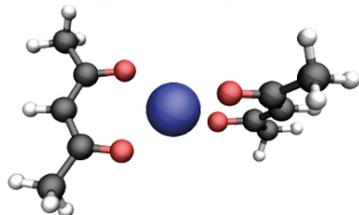
Ho	0.0016819728	-0.0012426710	-0.0035943216
C	3.7229882122	-1.7892500385	1.7832461819
C	2.9246594229	-0.8901146055	0.8878075483
O	1.6324388284	-0.9939987598	0.9879906761
C	3.5630956178	-0.0009445249	0.0039680344
C	2.9284331879	0.8880617264	-0.8828462568
C	3.7306987089	1.7879481454	-1.7740134700
O	1.6367144211	0.9914580780	-0.9890255878
H	3.4534520572	-1.5911682412	2.8269722007
H	4.7982515111	-1.6607429426	1.6559680135
H	3.4541736361	-2.8322346262	1.5803340309
H	4.6457326398	-0.0007228926	0.0065169453
H	4.8053974370	1.6574392786	-1.6440282723
H	3.4631551793	2.8309006360	-1.5690844985
H	3.4635908001	1.5930600328	-2.8189280159
C	-3.7347255800	-1.7751211086	-1.7808927379
C	-2.9312993279	-0.8815848790	-0.8842790882
O	-1.6398906618	-0.9859050667	-0.9904001827
C	-3.5646753369	0.0046167847	0.0060900692
C	-2.9232333533	0.8885746479	0.8927239464
C	-3.7182851918	1.7847973679	1.7940864250
O	-1.6307703118	0.9884594731	0.9915733818
H	-4.8092460128	-1.6406161055	-1.6534618078
H	-3.4722337697	-2.8198672464	-1.5785187776
H	-3.4638443794	-1.5780330049	-2.8244020229
H	-4.6473032591	0.0064274408	0.0092363004
H	-3.4537575444	2.8286716442	1.5898483540
H	-3.4416157102	1.5870904483	2.8359544920
H	-4.7939851934	1.6536690092	1.6732624400

m/z 381, [Ho(acac-H)2(H2O)]+, +0.0 kJ/mol
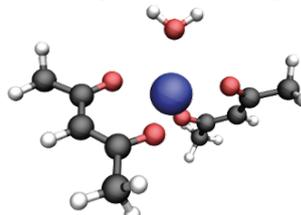
Ho	0.0000508356	-0.2886490514	-0.1497243965
C	3.0417653733	0.8267971387	2.9808287609
C	2.5738429158	0.4889756005	1.5952103086
O	1.3130109737	0.2005534247	1.4797404302
C	3.4651031390	0.4946068826	0.5112543356
C	3.1336194918	0.1769067564	-0.8216565480
C	4.1812619517	0.2334807583	-1.8980959559
O	1.9482188253	-0.1749441971	-1.1961667986
H	4.1087081823	1.0494462867	3.0198210131
H	2.8199679207	-0.0105209630	3.6520438386
H	2.4770958417	1.6891579469	3.3530446374
H	4.4934913549	0.7637574318	0.7165551903
H	5.1603283530	0.5264397694	-1.5171290774
H	3.8657178151	0.9448500268	-2.6697185935
H	4.2605983203	-0.7460582999	-2.3828330313
C	-4.1819639390	-1.4113627802	1.2875147051
C	-3.1339892015	-0.5663954175	0.6187168401
O	-1.9482646801	-1.0749231152	0.5504760066
C	-3.4653087047	0.7040972911	0.1053885022
C	-2.5739198333	1.5841662498	-0.5272847960
C	-3.0413126691	2.9101919001	-1.0528533586
O	-1.3132287475	1.3225480689	-0.6958461469
H	-5.1611265131	-0.9312995471	1.3051067764
H	-3.8671108325	-1.6286789217	2.3144722560
H	-4.2608433340	-2.3736826393	0.7693450753
H	-4.4936247125	1.0275541431	0.2059233478
H	-2.8200800630	2.9734396346	-2.1242318135
H	-2.4758941783	3.7122211471	-0.5648582940
H	-4.1080536579	3.0714484256	-0.8930795367
O	0.0011287680	-2.3980566222	-1.2297839314
H	0.7064821303	-2.7429332811	-1.7964325560
H	-0.7051221261	-3.0584210474	-1.1777341897

m/z 381, [Ho(acac-H)(acac-diketo)(OH)]+, +49.2 kJ/mol

m/z 381, [Ho(acac-H)(acac-enol)(OH)]+, +75.0 kJ/mol
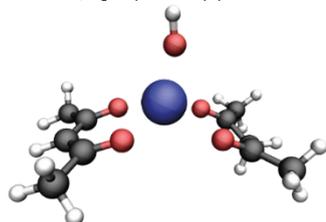
Ho	0.1160108815	0.0002802243	-0.5725745163
C	3.5616157231	-2.5254429942	0.9516752952
C	2.8239778496	-1.2479432204	0.6610736502
O	1.6243744393	-1.3781124496	0.2004880117
C	3.4337237522	-0.0012538753	0.8901409548
C	2.8251627640	1.2459986157	0.6610180612
C	3.5639610284	2.5228180658	0.9516508176
O	1.6257026014	1.3772609430	0.2003586568
H	4.5571115392	-2.3510084845	1.3622882481
H	3.6487540477	-3.1083063151	0.0277184240
H	2.9784522860	-3.1300685837	1.6549606244
H	4.4445455257	-0.0017257347	1.2781190787
H	4.5592935794	2.3474648875	1.3622683729
H	2.9813454343	3.1279529872	1.6549537609
H	3.6516334067	3.1056299637	0.0277131456
C	-3.7114637246	-2.5174125401	0.6910407604
C	-2.8328355201	-1.3068282653	0.6337192388
O	-1.6870739996	-1.3733888224	0.1891668211
C	-3.4123376709	0.0002555559	1.1648901385
C	-2.8323286325	1.3074973160	0.6347025682
C	-3.7105032997	2.5183678267	0.6928052684
O	-1.6865077632	1.3739438864	0.1902556794
H	-4.2265769581	-2.5854848157	1.6556191889
H	-3.1296900882	-3.4197022906	0.5004448086
H	-4.4916759869	-2.4233949327	-0.0770422537
H	-4.5023574153	0.0005095450	1.0629422672
H	-4.4906837207	2.4251856321	-0.0754132106
H	-3.1283823804	3.4205803283	0.5029053862
H	-4.2256805035	2.5859382999	1.6573845858
O	-0.0627244781	0.0004273954	-2.5675871342
H	0.0901937816	0.0007745954	-3.5149242158
H	-3.2320674983	-0.0001867440	2.2537075168

Ho	-0.3596230031	0.6347950718	0.0003491130
C	1.6654648818	-2.7549052429	0.0001632034
C	2.3924207811	-1.4413782892	0.0001584262
O	1.6804336776	-0.3564516454	0.0003120146
C	3.7966430499	-1.3936081073	-0.0000231019
C	4.5310126062	-0.2053127995	0.0000216641
C	6.0190861292	-0.1581117205	-0.0002357116
O	3.9558803754	0.9769790584	0.0003402360
H	1.0211590407	-2.8198602349	0.8851043523
H	2.3473275274	-3.6060573462	-0.0000015020
H	1.0208938105	-2.8197333029	-0.8845936769
H	4.3451392626	-2.3261419746	-0.0002152909
H	6.4574180883	-1.1559852412	-0.0004629989
H	6.3661799109	0.3948881556	0.8800606111
H	6.3658630249	0.3951486923	-0.8804935892
C	-3.7923731714	-0.8499764849	-2.5233052760
C	-3.0515578045	-0.5608259791	-1.2498606257
O	-1.8405432915	-0.1206759984	-1.3854163922
C	-3.6614676832	-0.7701125161	0.0002662124
C	-3.0514051173	-0.5613250764	1.2503979431
C	-3.7920685723	-0.8509443281	2.5238240106
O	-1.8403564624	-0.1212667707	1.3859770416
H	-4.7927788222	-1.2463719191	-2.3457488173
H	-3.2185099196	-1.5638572392	-3.1245327921
H	-3.8674638048	0.0714918585	-3.1120639290
H	-4.6787136159	-1.1407932242	0.0002541749
H	-3.8670067995	0.0702863280	3.1129731157
H	-3.2181783048	-1.5651180437	3.1246784594
H	-4.7925281848	-1.2471920309	2.3462413385
H	2.9771164775	0.8561435573	0.0005699841
O	-0.0790796939	2.6134055608	0.0007541972
H	-0.0746393926	3.5732622328	0.0009266053

m/z 395, [Ho(acac-H)2(MeOH)]+, +0.0 kJ/mol

m/z 395, [Ho(acac-H)(acac-diketo)(MeO)]+, +49.2 kJ/mol
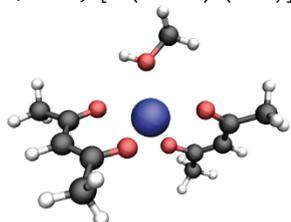
Ho	0.0210581515	0.1925650282	-0.0098658651
C	-2.9236824324	-2.1089054692	2.5116127520
C	-2.4896798253	-1.2828947665	1.3356614893
O	-1.2491262417	-0.9014774973	1.3400372488
C	-3.3905002559	-0.9617050020	0.3083081927
C	-3.0891387522	-0.1815059115	-0.8263496983
C	-4.1398060766	0.0805882531	-1.8688387112
O	-1.9285633118	0.3437657310	-1.0397101895
H	-3.9760415722	-2.3906678151	2.4597979795
H	-2.7421587806	-1.5478444002	3.4352058009
H	-2.3079704725	-3.0139768221	2.5646588841
H	-4.3998710421	-1.3435058185	0.3956901024
H	-5.1001064501	-0.3736073566	-1.6216192090
H	-3.7934976752	-0.3085713268	-2.8330866209
H	-4.2715146702	1.1613057277	-1.9922971825
C	4.2439151937	0.7119949490	1.6826590344
C	3.1841574420	0.1827934519	0.7562689899
O	1.9998199440	0.6783828749	0.9904893479
C	3.5064423277	-0.7954240249	-0.2053541849
C	2.6048507404	-1.3657237310	-1.1176205193
C	3.0638365295	-2.3835668238	-2.1212619277
O	1.3441227065	-1.0633857066	-1.1553173298
H	5.2177358501	0.2504331546	1.5145685856
H	3.9353057248	0.5386458758	2.7196938662
H	4.3338797685	1.7966608934	1.5540302740
H	4.5350801878	-1.1304711906	-0.2485045604
H	2.8307723770	-2.0267348457	-3.1307966710
H	2.5023624210	-3.3134872714	-1.9764473226
H	4.1320455380	-2.5913435549	-2.0483604922
C	-0.8391630975	3.6088111556	-0.3063581270
O	0.0689068234	2.5329313841	0.0687304509
H	-0.3428514951	4.2772745421	-1.0127613093
H	-1.1545319935	4.1518849175	0.5869835171
H	-1.6955940571	3.1331333106	-0.7818519501
H	0.8794774761	2.8828760854	0.4695513552

Ho	-0.1203169810	0.1030915354	0.4440133124
C	-3.3911973640	-2.7218343439	-0.9500180102
C	-2.7224963474	-1.3889025207	-0.7522681151
O	-1.5333381005	-1.4211611746	-0.2523614767
C	-3.3859588526	-0.1991003326	-1.1063308077
C	-2.8480304591	1.0932129902	-0.9732246753
C	-3.6393008475	2.2994052243	-1.3980973944
O	-1.6724284872	1.3265235841	-0.4921516323
H	-4.3808987688	-2.6325754497	-1.4001925120
H	-3.4791893930	-3.2268272922	0.0185876169
H	-2.7595658638	-3.3552199375	-1.5825313146
H	-4.3829713135	-0.2862664511	-1.5195427058
H	-4.6103888584	2.0368373021	-1.8202175890
H	-3.0642761000	2.8702646653	-2.1354755056
H	-3.7870794950	2.9556739567	-0.5329536157
C	3.7183807575	-2.5589026280	-0.5234635454
C	2.8306802082	-1.3554008841	-0.5982076741
O	1.7066354973	-1.3606285884	-0.0992789952
C	3.3744101949	-0.1336413412	-1.3354127545
C	2.8300670544	1.2325992831	-0.9326869508
C	3.7233850526	2.4159281556	-1.1369349016
O	1.6954465577	1.3630549986	-0.4725531915
H	4.1726487020	-2.7718999721	-1.4977072753
H	3.1585866741	-3.4226850122	-0.1638301746
H	4.5445115739	-2.3487685079	0.1696617690
H	4.4684541920	-0.1304444755	-1.3126111974
H	4.5398630349	2.3753479321	-0.4027951843
H	3.1655213661	3.3432526854	-1.0041093809
H	4.1915927119	2.3858495061	-2.1273443557
O	-0.0453235266	0.2810956164	2.4286683567
H	3.1112223398	-0.2712655938	-2.3982410662
C	-0.1928947229	0.4402575107	3.8217171616
H	0.5024526923	1.2019972329	4.1965405413
H	-1.2146421054	0.7526045415	4.0713763477
H	0.0164039771	-0.5045512152	4.3387298965

m/z 395, [Ho(acac-H)(acac-enol)(MeO)]+, +88.2 kJ/mol
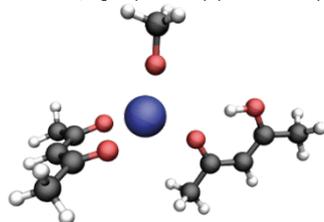
Ho	-0.3659773378	0.4953094719	-0.0041000044
C	1.6693197089	-2.8833442203	0.0093151723
C	2.4008645106	-1.5719562813	0.0052364340
O	1.6949658559	-0.4844847571	0.0010060259
C	3.8062268843	-1.5294212664	0.0059126161
C	4.5408560313	-0.3419594913	0.0024801674
C	6.0290824685	-0.2940057569	0.0033724267
O	3.9640693843	0.8399832318	-0.0018411928
H	1.0236646555	-2.9428765755	0.8936413747
H	2.3482164854	-3.7369070446	0.0133896599
H	1.0259014714	-2.9496462742	-0.8761732186
H	4.3527544394	-2.4630950201	0.0094219946
H	6.4676789530	-1.2917984735	0.0071340494
H	6.3753719253	0.2620526389	0.8820180636
H	6.3765905225	0.2559137562	-0.8786580234
C	-3.7800810504	-1.0558577065	-2.5222117457
C	-3.0407078210	-0.7491738227	-1.2513778522
O	-1.8406310692	-0.2833751685	-1.3922999901
C	-3.6437333203	-0.9699457756	0.0004765034
C	-3.0409939432	-0.7406460839	1.2509469682
C	-3.7806642864	-1.0388340694	2.5236333760
O	-1.8409979932	-0.2738168148	1.3890237938
H	-4.7721802460	-1.4710012059	-2.3407695869
H	-3.1944655414	-1.7604224764	-3.1230941598
H	-3.8746292777	-0.1378005770	-3.1134127944
H	-4.6525212279	-1.3630970127	0.0017064480
H	-3.8752945607	-0.1168761330	3.1087175517
H	-3.1952337580	-1.7394338850	3.1293193676
H	-4.7727385045	-1.4551320003	2.3447288600
H	2.9847390900	0.7142200226	-0.0021147746
O	-0.0773074718	2.4665266619	-0.0104463133
C	-0.0918148407	3.8798766735	-0.0152105046
H	0.4192317303	4.2672539404	0.8741509075
H	-1.1216493231	4.2567464066	-0.0176462975
H	0.4213164565	4.2613350891	-0.9059313025

m/z 423, [Ho(acac-H)2(CH3COOH-bonded)]+, +0.0 kJ/mol
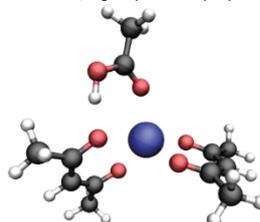
| Ho	0.1512831232	0.0333267787	-0.3803184239
C	-1.7893777261	-3.9581093684	-1.2662952963
C	-1.7349247564	-2.5883176407	-0.6543838735
O	-0.7207272949	-1.8593216918	-0.9757923343
C	-2.7537095202	-2.1462132209	0.2128489614
C	-2.8437909163	-0.8653533331	0.7719653787
C	-4.0203123663	-0.4895280483	1.6288526922
O	-1.9516652275	0.0642165929	0.5807518773
H	-1.7784087899	-3.8653743992	-2.3581500675
H	-2.6723451204	-4.5200314307	-0.9596145870
H	-0.8879604140	-4.5150980111	-0.9869365028
H	-3.5548111970	-2.8404360275	0.4326155596
H	-4.7118964751	-1.3202927283	1.7729956559
H	-4.5645492824	0.3437414348	1.1678192528
H	-3.6651489325	-0.1430238045	2.6058773861
C	4.5315844224	-0.1572862971	-1.5611509275
C	3.3642509848	-0.1485790222	-0.6166790776
C	3.5607613603	-0.2688359472	0.7743824058
C	2.5380605857	-0.2669738263	1.7333326884
C	2.8528866024	-0.3955495299	3.1960502292
O	1.2774057273	-0.1573476007	1.4383103683
O	2.1960806184	-0.0262941732	-1.1492803558
H	4.4139466627	-0.9831111995	-2.2718367215
H	5.4876074143	-0.2572320514	-1.0457260859
H	4.5293243684	0.7684143555	-2.1474691419
H	-2.3168554174	1.6542405888	0.5819420384
H	4.5787102142	-0.3676801416	1.1295028550
H	3.9234056809	-0.4787862803	3.3876176297
H	2.3425823556	-1.2773414464	3.5997287209
H	2.4548720142	0.4741457215	3.7308154370
C	-1.3693854975	3.0073728293	-0.3757607110
O	-2.3726582290	2.6436811521	0.3738739653
O	-0.4795451252	2.1934037075	-0.7278885337
C	-1.3254044266	4.4485402893	-0.7637957582
H	-0.7508168391	4.5743042770	-1.6817488364
H	-0.8223691391	5.0036824047	0.0377607765
H	-2.3339654417	4.8520150885	-0.8673386435

m/z 423, [Ho(acac-H)2(CH3COOH-cis)]+, +17.8 kJ/mol

m/z 423, [Ho(acac-H)(acac-diketo)(CH3COO)]+, +18.8 kJ/mol
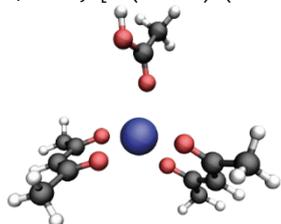
Ho	0.0200015570	0.0410981268	-0.0248524850
C	-3.9557877557	-1.0833588739	-1.9702981166
C	-2.9371885039	-1.0170004142	-0.8655899497
O	-1.8651321460	-0.3490736210	-1.1150570857
C	-3.1747165916	-1.6607065581	0.3658692227
C	-2.2920824034	-1.6480680100	1.4565071637
C	-2.6453388879	-2.3435627955	2.7411289832
O	-1.1417966648	-1.0528539662	1.4365046660
H	-4.2432759534	-0.0671327005	-2.2617120825
H	-4.8473791399	-1.6444853294	-1.6868464803
H	-3.4998279388	-1.5496721455	-2.8509519945
H	-4.1091747137	-2.1949939957	0.4825523794
H	-3.6281478029	-2.8156126127	2.7049830242
H	-2.6190272492	-1.6206854697	3.5640966522
H	-1.8864548512	-3.1027730447	2.9614134605
C	3.0472052290	-2.4346840590	-2.2933856330
C	2.5753123957	-1.5532584536	-1.1711874609
C	3.4365829060	-1.2074883420	-0.1185724289
C	3.0877779611	-0.3742574325	0.9634251656
C	4.0911269324	-0.0590790675	2.0386511814
O	1.9216064939	0.1554851012	1.0957130922
O	1.3468156777	-1.1506408323	-1.2507340554
H	2.4177717101	-3.3305946866	-2.3380110757
H	4.0907611316	-2.7321813700	-2.1814886423
H	2.9189197255	-1.9091196133	-3.2461824322
H	-1.2700968974	4.6271528850	1.1735762832
H	4.4438050686	-1.6039103440	-0.1438930772
H	5.0621014831	-0.5216745625	1.8560941918
H	3.7025193575	-0.4026988247	3.0039469543
H	4.2145918522	1.0269396196	2.1137954269
C	-0.3990334922	3.4836278754	-0.1081112473
O	-1.0560405432	3.6913290962	1.0266963659
O	-0.0813126282	2.3239645872	-0.3777442513
C	-0.0796254171	4.6516955809	-0.9928957421
H	0.4481775361	4.3106957382	-1.8824390611
H	0.5453690555	5.3718661289	-0.4525470779
H	-1.0023344925	5.1626723856	-1.2902998338

|			
Ho	0.1638859698	0.2481627694	-0.0542817104
C	3.9802191657	0.0897436749	2.3657650273
C	3.1190411700	-0.1470734238	1.1578941660
O	1.8754100912	0.1901565110	1.2722004399
C	3.6595334233	-0.7019053342	-0.0144766585
C	2.9330842743	-0.9553571622	-1.1926177577
C	3.6098758219	-1.5464599093	-2.3971518606
O	1.6719418312	-0.7031756486	-1.3163700720
H	3.9668484548	1.1570518531	2.6142578336
H	5.0114830109	-0.2317765416	2.2141889268
H	3.5550093523	-0.4420017899	3.2241683691
H	4.7131654245	-0.9509759518	-0.0114708845
H	4.6656557431	-1.7589137615	-2.2236027713
H	3.5143469084	-0.8517555470	-3.2394006259
H	3.0950313208	-2.4692501233	-2.6864871558
C	-2.8182891382	-2.3252678926	2.5328073105
C	-2.2796755293	-1.5047791830	1.4047572791
C	-3.2577042381	-1.0116384050	0.3465722033
C	-2.7390587653	-1.0779104123	-1.0859463471
C	-3.6886678277	-1.5154904646	-2.1558058781
O	-1.5782957263	-0.7597521081	-1.3516506327
O	-1.0821490232	-1.2173871598	1.3386400192
H	-2.0353096852	-2.5391206369	3.2605115963
H	-3.2320164750	-3.2633520681	2.1404908937
H	-3.6499373761	-1.7964706582	3.0147662379
H	-3.3991049271	0.0628704927	0.5590818122
H	-4.2273529768	-1.5038240032	0.4413717644
H	-3.9865638631	-2.5569455916	-1.9770312495
H	-3.2266854765	-1.4259460492	-3.1391759406
H	-4.6073405534	-0.9178000938	-2.1105691233
C	-1.0612444443	2.6433893270	-0.0850311514
O	0.0210688985	2.3894893854	-0.7325345705
O	-1.6096405041	1.6997004238	0.5822107919
C	-1.6370479943	4.0280253611	-0.1100496332
H	-2.6306922013	4.0483560618	0.3378068544
H	-1.6645045883	4.3999340598	-1.1378028780
H	-0.9728275471	4.6930519996	0.4532273755

m/z 423, [Ho(acac-H)2(CH3COOH-trans)]+, +26.3 kJ/mol
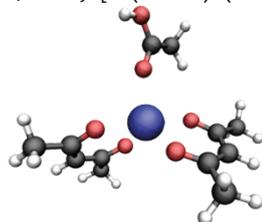
Ho	0.0622494384	0.0511943679	-0.0978012633
C	3.1181919372	-1.1186225037	3.0108076642
C	2.6607897285	-0.6960372282	1.6436178810
O	1.3895035483	-0.4645586018	1.5218193258
C	3.5729716723	-0.5670010417	0.5872371440
C	3.2386511650	-0.1598459718	-0.7218674309
C	4.3015616483	-0.0446031829	-1.7789703705
O	2.0380669515	0.1321229037	-1.0829402095
H	2.8388313111	-0.3507892048	3.7408905826
H	4.1948140850	-1.2875860472	3.0577778138
H	2.5943907918	-2.0368236870	3.2997234569
H	4.6126521386	-0.7874748514	0.7938128095
H	5.2964022126	-0.2875335291	-1.4032010364
H	4.3041401835	0.9742326170	-2.1818669577
H	4.0549968714	-0.7145563576	-2.6103760523
C	-3.9590088184	-1.0020230725	1.8095595922
C	-2.8383861147	-1.1104983000	0.8114710722
C	-2.8477973407	-2.1308799185	-0.1593916010
C	-1.8540871067	-2.3235243535	-1.1324230982
C	-1.9714619092	-3.4281554111	-2.1441017768
O	-0.7936570178	-1.5859991655	-1.2232380219
O	-1.9024227607	-0.2277754386	0.9028793057
H	-3.5458893433	-1.0586768843	2.8227871727
H	-4.7108421406	-1.7821974928	1.6830694276
H	-4.4403151863	-0.0220820316	1.7142585027
H	-0.3414163598	4.1539290943	-1.7796165208
H	-3.6873214576	-2.8145648581	-0.1599693218
H	-2.8883340809	-4.0074094997	-2.0271394943
H	-1.1068543960	-4.0952387712	-2.0530359837
H	-1.9373289662	-3.0009320892	-3.1524917082
C	-1.0904525953	3.3173712531	-0.2533477223
O	-0.9713484526	4.3514045692	-1.0618142903
O	-0.4582372362	2.2690178518	-0.4649821674
C	-2.0036443210	3.5375463031	0.9077130069
H	-2.3069774586	2.5809380808	1.3337968348
H	-2.8704374657	4.1285995027	0.6041622802
H	-1.4628101554	4.1154629502	1.6672931545

m/z 423, [Ho(acac-H)(acac-enol)(CH3COO)]+, +36.1 kJ/mol
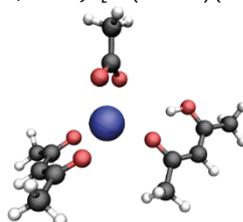
Ho	0.4196218240	0.3020215683	-0.0862936010
C	-0.0881447216	2.8857244549	-0.3910107980
O	0.6286831319	2.2232476267	-1.2327094233
O	-0.5852083142	2.2572283329	0.6091410950
C	-0.3034041426	4.3566260878	-0.5721499641
H	-1.1854426259	4.6873586067	-0.0227230669
H	-0.3806123678	4.6008027958	-1.6335789838
H	0.5722547133	4.8835632230	-0.1743458884
C	3.7561508053	-0.7465462826	2.7535485130
C	3.0360059076	-0.7523213480	1.4366724978
O	1.8724465135	-0.1780862310	1.4255326230
C	3.6068819601	-1.3512154746	0.3024741126
C	2.9922989258	-1.4322622322	-0.9619634258
C	3.6843072874	-2.1107206445	-2.1092540419
O	1.8217012638	-0.9425980657	-1.2084446317
H	3.9127541212	0.2895303246	3.0747376568
H	4.7177105246	-1.2591439271	2.7064157790
H	3.1264765420	-1.2216315063	3.5140768319
H	4.5866790881	-1.7983570057	0.4129480972
H	4.6509822973	-2.5300880969	-1.8276332362
H	3.8265561361	-1.3867219361	-2.9198082685
H	3.0429450342	-2.9064332339	-2.5039534686
C	-1.6112891571	-3.0337193545	-0.8274348057
C	-2.2963612896	-1.7913043119	-0.3385931198
O	-1.5633545172	-0.7465914619	-0.1110434476
C	-3.6857186183	-1.7670191537	-0.1286893682
C	-4.3869576671	-0.6509690163	0.3321172629
C	-5.8606916528	-0.6437316514	0.5481950697
O	-3.8024442086	0.4924330274	0.6147852845
H	-1.0164376764	-2.8043692778	-1.7185714197
H	-2.3178924150	-3.8303349988	-1.0629105089
H	-0.9192291558	-3.3945902715	-0.0567031231
H	-4.2521265739	-2.6654134220	-0.3352053538
H	-6.3117767259	-1.6058999154	0.3061391829
H	-6.3156812644	0.1398221840	-0.0683757116
H	-6.0743617190	-0.3907454889	1.5929117219
H	-2.8340752631	0.4197860765	0.4542489282

m/z 463, [Ho(acac-H)2(acac-diketo)]+, +0.0 kJ/mol

m/z 463, [Ho(acac-H)2(acac-enol)]+, +10.1 kJ/mol
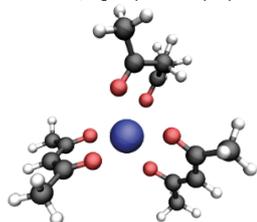
Ho	-0.2066947606	0.0717275432	0.1575817321
C	-3.8085595192	0.5349986070	-2.5656799539
C	-3.0855750012	0.1242232614	-1.3115880523
O	-1.8157751692	0.3529943095	-1.2920930726
C	-3.7866218244	-0.4657870834	-0.2452225139
C	-3.2048623222	-0.8818693173	0.9676047672
C	-4.0540043850	-1.4937110354	2.0491326499
O	-1.9479542585	-0.7692504879	1.2258979016
H	-3.6745408899	1.6111242898	-2.7230336394
H	-4.8747609989	0.3063569050	-2.5299154481
H	-3.3569644048	0.0290152836	-3.4261456860
H	-4.8535500916	-0.6070563679	-0.3643031365
H	-5.1038805750	-1.5753672036	1.7636826683
H	-3.9725890007	-0.8857630289	2.9571878573
H	-3.6665476129	-2.4883303795	2.2960380142
C	3.2009625143	2.2895610020	-2.0202267458
C	2.1093921919	2.0949510001	-0.9980371224
O	1.5912126930	0.9160725513	-0.9372467990
C	1.7202558119	3.1704609792	-0.1785205920
C	0.7200253921	3.1102202388	0.8090495420
C	0.4148791718	4.3092843088	1.6643184708
O	0.0174701464	2.0554028848	1.0397782261
H	3.6036948064	3.3035659087	-2.0188451644
H	2.8051622271	2.0617413789	-3.0162562774
H	4.0167965408	1.5828617200	-1.8291746046
H	2.2381218510	4.1124553425	-0.3086949120
H	0.5352968728	4.0406751420	2.7196459834
H	-0.6346814746	4.5925479963	1.5268327430
H	1.0524967162	5.1637339522	1.4327010156
C	1.7672071187	-3.7079347954	-1.9595703847
C	1.5767384540	-2.5475903968	-1.0331097045
C	2.7535164204	-2.1313458363	-0.1537268059
C	2.3705774101	-1.8048132276	1.2864399456
C	3.2357133773	-2.3369421639	2.3857894090
O	1.3844198125	-1.1080348774	1.5260590113
O	0.5152979786	-1.9286845700	-0.9874469724
H	0.8821414812	-3.8514175064	-2.5796866439
H	1.9683010443	-4.6163828994	-1.3773543828
H	2.6485103139	-3.5411329240	-2.5911808418
H	3.1185069348	-1.1860803930	-0.5898948086
H	3.5630620911	-2.8620506799	-0.1962722748
H	3.2113014950	-3.4343454384	2.3735535467
H	2.8950974158	-1.9689045007	3.3537964611
H	4.2800450052	-2.0475444921	2.2156225945
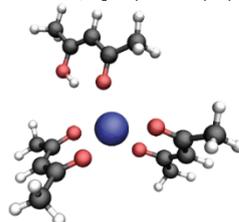
Ho	-0.4736656948	0.0183047207	0.0780536799
C	-1.3346166482	3.8636118698	2.3027174517
C	-0.6737297373	3.0180976758	1.2501932332
O	-0.9568374564	1.7553383449	1.2829600320
C	0.1916207554	3.5942068107	0.3065614763
C	0.8821436323	2.8828788497	-0.6948935499
C	1.7987335023	3.6026980722	-1.6459651495
O	0.7806938626	1.6078369366	-0.8538198634
H	-2.4226182834	3.7741621876	2.2076432218
H	-1.0515933975	4.9149029816	2.2342330808
H	-1.0701895295	3.4798465447	3.2943665681
H	0.3514902555	4.6636269969	0.3623360375
H	1.8634383066	4.6718581359	-1.4390229411
H	1.4397522516	3.4545941291	-2.6708210379
H	2.7995500164	3.1602237918	-1.5922441563
C	-3.6062943604	-2.9225897676	1.6322116592
C	-2.9261129773	-2.0475784771	0.6148256675
O	-1.8384513805	-1.4696127909	0.9928036253
C	-3.4761675674	-1.8925912843	-0.6735060940
C	-2.9215691294	-1.1040099556	-1.6942366114
C	-3.5739803464	-1.0272653096	-3.0461355087
O	-1.8406243923	-0.4061555082	-1.5501931427
H	-4.5063442450	-3.3996923650	1.2418673412
H	-3.8690961188	-2.3174136352	2.5072456406
H	-2.9079006529	-3.6932006958	1.9767435406
H	-4.3902199561	-2.4285089331	-0.8962871884
H	-2.8572035468	-1.3414818374	-3.8129544965
H	-3.8339966297	0.0149344571	-3.2630606402
H	-4.4708873696	-1.6444584964	-3.1141938371
O	3.6906868731	0.0749983127	-0.6334773605
C	4.2951412968	-1.0089149927	-0.1913293629
H	6.2183662929	-0.1398570383	0.0551708662
H	5.9626197139	-0.9177812493	-1.5044133668
C	5.7668343456	-1.0123365294	-0.4303760140
H	6.2368136019	-1.9209180630	-0.0539995395
C	3.6233196873	-2.0525848851	0.4405363489
H	4.2083304234	-2.9016241926	0.7685575887
C	2.2331431564	-2.0633365184	0.6764406926
O	1.4897915007	-1.0767608872	0.3079388151
C	1.5760778095	-3.2293574110	1.3560161402
H	0.9648406351	-2.8759540737	2.1931247203
H	0.8984231184	-3.7232505877	0.6492122783
H	2.3007939114	-3.9599570593	1.7173615532
H	2.7226484704	0.0221927262	-0.4560723984