

IR and Raman Characterization of the Zincocenes ($\eta^5\text{-C}_5\text{Me}_5$)₂Zn₂ and ($\eta^5\text{-C}_5\text{Me}_5$)($\eta^1\text{-C}_5\text{Me}_5$)Zn

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Supporting Information

Results of quantum chemical calculations

1. Zn₂Cp*₂: Calculation of the structure, vibrational spectrum (IR intensities), potential energy distribution

Program package: TURBOMOLE

Basis sets: 6311+G**

DFT model: B3-LYP_Gaussian

a) Zn₂Cp*₂ (Tables S1 and S2)

Total energy: -4339.1224314550 a.u.

Calculated structural parameters (symmetry D_{5h} , definition as in Table 3 of the main text):

$$k_1 = r(\text{Zn}-\text{C}_1) = 2.311 \text{ \AA}$$

$$k_2 = r(\text{C}_1-\text{C}_{1a}) = 1.504 \text{ \AA}$$

$$k_3 = r(\text{C}_{1a}-\text{H}_{1a}) = 1.097 \text{ \AA}$$

$$k_4 = r(\text{C}_{1a}-\text{H}_{1b}) = 1.093 \text{ \AA}$$

$$k_5 = r(\text{Zn}-\text{Zn}') = 2.338 \text{ \AA}$$

$$k_6 = r(\text{C}_1-\text{C}_2) = 1.433 \text{ \AA}$$

$$k_7 = \angle(\text{Zn}-\text{C}_1-\text{C}_{1a}) = 125.9^\circ$$

$$k_8 = \angle(\text{C}_1-\text{C}_{1a}-\text{H}_{1a}) = 111.2^\circ$$

$$k_9 = \angle(\text{C}_1\text{-C}_{1\text{a}}\text{-H}_{1\text{b}}) = 111.9^\circ$$

$$k_{10} = \angle(\text{H}_{1\text{b}}\text{-C}_{1\text{a}}\text{-H}_{1\text{c}}) = 107.4^\circ$$

2. Zn_2Cp^*_2 , ZnCp^*_2 : Calculation of the structures, vibrational spectra (IR, Raman intensities)

Program package: Gaussian 03

Basis sets: Zn, C (Cp) : 6311+G*

C (Methyl), H : 631+G**

DFT model: B3-LYP

a) Zn_2Cp^*_2 (Tables S3 and S4)

Total energy: -4339.04151493 a.u.

Calculated structural parameters (symmetry D_{5h} , definition as in Table 3 of the main text):

$$k_1 = r(\text{Zn-C}_1) = 2.313 \text{ \AA}$$

$$k_2 = r(\text{C}_1\text{-C}_{1\text{a}}) = 1.503 \text{ \AA}$$

$$k_3 = r(\text{C}_{1\text{a}}\text{-H}_{1\text{a}}) = 1.099 \text{ \AA}$$

$$k_4 = r(\text{C}_{1\text{a}}\text{-H}_{1\text{b}}) = 1.095 \text{ \AA}$$

$$k_5 = r(\text{Zn-Zn}') = 2.338 \text{ \AA}$$

$$k_6 = r(\text{C}_1\text{-C}_2) = 1.433 \text{ \AA}$$

$$k_7 = \angle(\text{Zn-C}_1\text{-C}_{1\text{a}}) = 126.1^\circ$$

$$k_8 = \angle(\text{C}_1\text{-C}_{1\text{a}}\text{-H}_{1\text{a}}) = 111.2^\circ$$

$$k_9 = \angle(\text{C}_1\text{-C}_{1\text{a}}\text{-H}_{1\text{b}}) = 111.9^\circ$$

$$k_{10} = \angle(\text{H}_{1\text{b}}\text{-C}_{1\text{a}}\text{-H}_{1\text{c}}) = 107.4^\circ$$

b) ZnCp^*_2 (Tables S5 and S6)

Total energy: = -2559.6564214 a.u.

Selected calculated structural parameters (symmetry C_1):

$$r(\text{Zn}-\text{C}(\eta^5\text{-Cp})) = 2.264\text{-}2.321 \text{ \AA}$$

$$r(\text{Zn}-\text{C}(\eta^1\text{-Cp})) = 2.023, 2.738\text{-}3.474 \text{ \AA}$$

$$r(\text{C}-\text{C})(\eta^5\text{-Cp}) = 1.433\text{-}1.436 \text{ \AA}$$

$$r(\text{C}-\text{C})(\eta^1\text{-Cp}) = 1.368, 1.463, 1.493 \text{ \AA}$$

$$r(\text{C}(\eta^5\text{-Cp})-\text{C}(\text{Me})) = 1.504 \text{ \AA}$$

$$r(\text{C}(\eta^1\text{-Cp})-\text{C}(\text{Me})) = 1.368, 1.463, 1.493 \text{ \AA}$$

Table S1: Vibrational spectrum of Zn_2Cp^*_2 (module NumForce, TURBOMOLE)

Table S2: Potential energy distributions of the modes of the a_1' and a_2'' irreducible representations of Zn_2Cp^*_2 (module aoforce, TURBOMOLE)

Table S3: Calculated structural parameters (\AA) of Zn_2Cp^*_2 (Gaussian 03):

Table S4: Vibrational spectrum of Zn_2Cp^*_2 (Gaussian 03):

Table S5: Calculated structural parameters (\AA) of ZnCp^*_2 (Gaussian 03):

Table S6: Vibrational spectrum of ZnCp^*_2 (Gaussian 03):

Table S1: Vibrational spectrum of Zn_2Cp^*_2 (module NumForce, TURBOMOLE)

mode	symmetry	ν (cm^{-1}) $^{(\text{nat})}\text{Zn}_2\text{Cp}^*_2$	ν (cm^{-1}) $^{68}\text{Zn}_2\text{Cp}^*_2$	IR intensity (km/mole)
1		0	0.00	
2		0	0.00	0.00
3		0	0.00	0.00
4		0	0.00	0.00
5		0	0.00	0.00
6		0	0.00	0.00
7	e_1'	27.24	27.05	0.00
8	e_1'	27.24	27.05	0.37
9	a_1''	51.13	51.13	0.37
10	e_1''	53.64	52.78	0.00
11	e_1''	53.64	52.78	0.00
12	e_1''	96.22	96.00	0.00
13	e_1''	96.22	96.00	0.00
14	e_1'	102.33	101.71	0.00
15	e_1'	102.33	101.71	0.50
16	a_1'	107.37	107.30	0.50
17	e_2''	149.93	149.93	0.00
18	e_2''	149.93	149.93	0.00
19	e_2'	150.81	150.81	0.00
20	e_2'	150.81	150.81	0.00
21	e_2''	153.66	153.66	0.00
22	e_2''	153.66	153.66	0.00
23	e_2'	153.90	153.90	0.00
24	e_2'	153.90	153.90	0.00
25	a_2''	157.76	156.57	0.00
26	e_1''	163.06	163.06	0.02
27	e_1''	163.06	163.06	0.00
28	a_2'	165.25	165.25	0.00

29	a_1''	167.22	167.22	0.00
30	e_1'	167.23	167.22	0.00
31	e_1'	167.23	167.22	0.07
32	a_1'	228.59	226.94	0.07
33	e_1'	284.36	284.36	0.00
34	e_1'	284.36	284.36	2.32
35	e_1''	286.09	286.09	2.32
36	e_1''	286.09	286.09	0.00
37	e_2''	298.35	298.35	0.00
38	e_2''	298.35	298.35	0.00
39	e_2'	299.36	299.36	0.00
40	e_2'	299.36	299.36	0.00
41	a_2''	318.25	316.46	0.00
42	e_1'	347.33	347.33	260.62
43	e_1'	347.33	347.33	0.20
44	e_1''	365.58	365.54	0.20
45	e_1''	365.58	365.54	0.00
46	a_1'	381.81	377.35	0.00
47	e_2'	550.96	550.96	0.00
48	e_2'	550.96	550.96	0.00
49	e_2''	551.14	551.14	0.00
50	e_2''	551.14	551.14	0.00
51	a_2'	560.36	560.36	0.00
52	a_1''	560.72	560.72	0.00
53	a_2''	590.93	590.93	0.00
54	a_1'	592.76	592.76	12.38
55	e_2''	630.98	630.98	0.00
56	e_2''	630.98	630.98	0.00
57	e_2'	639.52	639.52	0.00
58	e_2'	639.52	639.52	0.00
59	e_1''	807.21	807.20	0.00
60	e_1''	807.21	807.20	0.00

61	e_1'	808.56	808.56	0.00
62	e_1'	808.56	808.56	3.45
63	e_2''	959.86	959.86	3.45
64	e_2''	959.86	959.86	0.00
65	e_2'	960.28	960.28	0.00
66	e_2'	960.28	960.28	0.00
67	e_1''	1043.22	1043.22	0.00
68	e_1''	1043.22	1043.22	0.00
69	e_1'	1045.09	1045.09	0.00
70	e_1'	1045.09	1045.09	16.57
71	a_1'	1053.01	1053.01	16.57
72	a_2''	1054.19	1054.19	0.00
73	e_2'	1054.66	1054.66	0.21
74	e_2'	1054.66	1054.66	0.00
75	e_2''	1056.45	1056.45	0.00
76	e_2''	1056.45	1056.45	0.00
77	e_1''	1081.68	1081.68	0.00
78	e_1''	1081.68	1081.68	0.00
79	e_1'	1081.69	1081.69	0.00
80	e_1'	1081.69	1081.69	2.54
81	a_2'	1121.94	1121.94	2.54
82	a_1''	1122.40	1122.40	0.00
83	e_2''	1178.85	1178.85	0.00
84	e_2''	1178.85	1178.85	0.00
85	e_2'	1179.65	1179.65	0.00
86	e_2'	1179.65	1179.65	0.00
87	e_2''	1400.62	1400.62	0.00
88	e_2''	1400.62	1400.62	0.00
89	e_2'	1401.06	1401.06	0.00
90	e_2'	1401.06	1401.06	0.00
91	a_2''	1416.02	1416.02	0.00
92	e_1''	1416.26	1416.26	51.05

93	e_1''	1416.26	1416.26	0.00
94	e_1'	1416.73	1416.73	0.00
95	e_1'	1416.73	1416.73	5.20
96	a_1'	1417.01	1417.01	5.20
97	e_2''	1420.24	1420.24	0.00
98	e_2''	1420.24	1420.24	0.00
99	e_2'	1420.37	1420.37	0.00
100	e_2'	1420.37	1420.37	0.00
101	a_2''	1441.63	1441.63	0.00
102	a_1'	1441.82	1441.82	8.42
103	e_1''	1462.26	1462.25	0.00
104	e_1''	1462.26	1462.25	0.00
105	e_1'	1464.58	1464.58	0.00
106	e_1'	1464.58	1464.58	15.82
107	e_2''	1480.94	1480.94	15.82
108	e_2''	1480.94	1480.94	0.00
109	e_2'	1482.99	1482.99	0.00
110	e_2'	1482.99	1482.99	0.00
111	a_2'	1488.23	1488.23	0.00
112	a_1''	1488.81	1488.81	0.00
113	e_1''	1489.29	1489.29	0.00
114	e_1''	1489.29	1489.29	0.00
115	e_1'	1490.69	1490.69	0.00
116	e_1'	1490.69	1490.69	0.19
117	a_2''	1501.51	1501.51	0.19
118	a_1'	1502.62	1502.61	62.88
119	e_2''	1509.38	1509.38	0.00
120	e_2''	1509.38	1509.38	0.00
121	e_2'	1510.03	1510.03	0.00
122	e_2'	1510.03	1510.03	0.00
123	e_1''	1516.97	1516.97	0.00
124	e_1''	1516.97	1516.97	0.00

125	e_1'	1518.82	1518.82	0.00
126	e_1'	1518.82	1518.82	27.83
127	e_1''	3002.38	3002.38	27.83
128	e_1''	3002.38	3002.38	0.00
129	e_2'	3002.50	3002.50	0.00
130	e_2'	3002.50	3002.50	0.00
131	e_1'	3002.73	3002.73	0.00
132	e_1'	3002.73	3002.73	243.21
133	e_2''	3002.86	3002.86	243.21
134	e_2''	3002.86	3002.86	0.00
135	a_2''	3005.08	3005.08	0.00
136	a_1'	3006.93	3006.93	210.72
137	a_1'	3061.18	3061.18	0.00
138	e_2''	3062.67	3062.67	0.00
139	e_2''	3062.67	3062.67	0.00
140	e_1''	3063.85	3063.85	0.00
141	e_1''	3063.85	3063.85	0.00
142	e_1'	3064.04	3064.04	0.00
143	e_1'	3064.04	3064.04	52.16
144	e_2'	3064.77	3064.77	52.16
145	e_2'	3064.77	3064.77	0.00
146	a_2''	3065.85	3065.85	0.00
147	a_2'	3090.04	3090.04	77.22
148	a_1''	3092.46	3092.46	0.00
149	e_1''	3095.44	3095.44	0.00
150	e_1''	3095.44	3095.44	0.00
151	e_1'	3095.99	3095.99	0.00
152	e_1'	3095.99	3095.99	91.95
153	e_2''	3098.26	3098.26	91.95
154	e_2''	3098.26	3098.26	0.00
155	e_2'	3099.34	3099.34	0.00
156	e_2'	3099.34	3099.34	0.00

Table S2: Potential energy distributions of the modes of the a_1' and a_2'' irreducible representations of $Zn_2Cp^*_2$ (module aoforce, TURBOMOLE)

ν (cm^{-1})	symmetry coordinate	potential energy distribution*	
		V_{ii}^n (diagonal)	V^n (brutto)
107.37	1	4.964328	0.411856
	5	0.219519	0.283080
	7	1.090397	0.287010
157.76	11	7.295086	0.399357
	16	2.627443	0.569646
	17	0.136033	0.005797
	18	0.086274	0.005486
228.59	1	0.084976	0.001215
	5	0.509409	0.476602
	7	2.886983	0.498421
	8	0.170048	0.010209
	9	0.066340	0.005526
318.25	11	16.874066	0.589022
	16	2.885989	0.384642
	17	0.239041	0.016353
	18	0.074417	0.006622
381.81	1	12.688727	0.575367
	5	0.307193	0.240332

	7	1.356654	0.168324
	8	0.110433	0.009720
590.93	12	2.521926	0.539838
	15	1.263502	0.448479
	16	0.051622	0.009269
592.76	2	2.525246	0.541344
	6	1.259081	0.441412
	7	0.060912	0.014698
1053.01	1	0.087664	0.002966
	7	0.110681	0.030261
	8	4.158479	0.523917
	9	2.696697	0.372077
	10	0.337362	0.072155
1054.19	11	0.086870	0.001087
	16	0.110668	0.035526
	17	4.120566	0.518879
	18	2.697246	0.372923
	19	0.341949	0.073000
1416.02	11	0.102135	0.005323
	12	0.486539	0.136408
	15	0.822064	0.245688
	17	0.744127	0.214974

	18	1.940756	0.421738
	19	0.521171 -	0.023831
1417.01	1	0.095262	0.003431
	2	0.436442	0.125609
	6	0.791976	0.236240
	8	0.757081	0.217657
	9	2.058543	0.440282
	10	0.583765 -	0.022583
1441.63	11	0.097493	0.002803
	12	2.193509	0.311965
	15	0.904176	0.281439
	17	0.788415	0.182160
	18	1.272350	0.249523
	19	0.102311 -	0.028209
1441.82	1	0.101835	0.002524
	2	2.240517	0.320278
	6	0.956449	0.294945
	8	0.745694	0.170423
	9	1.234332	0.238531
	10	0.108999 -	0.027581
1501.51	12	0.068144	0.009317
	17	0.140500	0.064190
	18	0.720209 -	0.056690
	19	5.404446	0.979152

1502.62	2	0.065337	0.009534
	8	0.153085	0.069082
	9	0.664101 -	0.061109
	10	5.356598	0.978411
3005.08	13	4.229744	0.848559
	14	1.461183	0.153497
3006.93	3	4.236013	0.850757
	4	1.438269	0.151320
3061.18	3	0.796642	0.151586
	4	8.540888	0.849907
3065.85	13	0.805081	0.153827
	14	8.492587	0.847929

* Potential energy contributions V_{ij}^n , defined as $V_{ij}^n = (L_i^n L_j^n F_{ij})/v^n$, where L_i^n are the elements of the normal coordinates belonging to mode n, and F_{ij} are the elements of the force constant matrix, both expressed in the basis system of symmetry coordinates; v^n is the related vibrational frequency.

Diagonal contributions $V_{ii}^n = (L_i^n L_i^n F_{ii})/v^n$.

Brutto contributions $V^n = \sum_i (L_i^n L_j^n F_{ij})/v^n$.

Table S3: Calculated structural parameters (Å) of Zn₂Cp*₂ (Gaussian 03):

No.	Atom	x	y	z
1	Zn	0.000	0.000	1.169
2	Zn	0.000	0.000	-1.169
3	C	-0.717	-0.986	3.134
4	C	-1.159	0.377	3.134
5	C	0.000	1.219	3.134
6	C	1.159	0.377	3.134
7	C	0.717	-0.986	3.134
8	C	-1.159	0.377	-3.134
9	C	-0.717	-0.986	-3.134
10	C	0.717	-0.986	-3.134
11	C	1.159	0.377	-3.134
12	C	0.000	1.219	-3.134
13	C	0.000	2.718	3.248
14	H	0.882	3.163	2.777
15	H	0.000	3.037	4.300
16	H	-0.882	3.163	2.777
17	C	-2.585	0.840	3.248
18	H	-2.735	1.817	2.777
19	H	-2.889	0.939	4.300
20	H	-3.281	0.138	2.777
21	C	-1.598	-2.199	3.248
22	H	-1.785	-2.457	4.300
23	H	-1.145	-3.077	2.777
24	H	-2.573	-2.040	2.777
25	C	2.585	0.840	3.248
26	H	2.735	1.817	2.777
27	H	3.281	0.138	2.777
28	H	2.889	0.939	4.300
29	C	1.598	-2.199	3.248

30	H	2.573	-2.040	2.777
31	H	1.145	-3.077	2.777
32	H	1.785	-2.457	4.300
33	C	-1.598	-2.199	-3.248
34	H	-1.785	-2.457	-4.300
35	H	-2.573	-2.040	-2.777
36	H	-1.145	-3.077	-2.777
37	C	-2.585	0.840	-3.248
38	H	-3.281	0.138	-2.777
39	H	-2.889	0.939	-4.300
40	H	-2.735	1.817	-2.777
41	C	0.000	2.718	-3.248
42	H	-0.882	3.163	-2.777
43	H	0.000	3.037	-4.300
44	H	0.882	3.163	-2.777
45	C	2.585	0.840	-3.248
46	H	2.889	0.939	-4.300
47	H	3.281	0.138	-2.777
48	H	2.735	1.817	-2.777
49	C	1.598	-2.199	-3.248
50	H	1.145	-3.077	-2.777
51	H	2.573	-2.040	-2.777
52	H	1.785	-2.457	-4.300

Table S4: Vibrational spectrum of Zn₂Cp*₂ (Gaussian 03):

ν (cm ⁻¹)	IR intensity (km/mole)	Raman intensity (Å ⁴ /amu)
-13.83	0.00	0.00
22.54	0.05	0.01
23.21	0.05	0.00
48.38	0.00	2.23
48.62	0.00	2.41
91.79	0.00	8.09
92.58	0.00	6.44
94.00	0.00	14.35
96.77	0.00	1.44
102.09	0.74	0.03
103.11	0.75	0.08
107.21	0.01	2.47
113.33	0.00	0.07
117.78	0.00	0.59
119.38	0.00	0.01
120.92	0.01	3.26
123.53	0.00	0.52
125.21	0.04	0.31
126.86	0.01	0.44
131.01	0.05	0.04
145.93	0.00	0.00
147.85	0.00	0.02
147.98	0.00	0.00
150.42	0.00	0.03
157.04	0.01	0.00
228.82	0.00	1.65
280.97	0.00	0.18
281.00	2.45	0.00

284.40	0.02	0.24
284.41	2.42	0.01
292.05	0.00	0.00
292.43	0.00	0.53
294.15	0.00	0.00
294.40	0.02	0.49
316.26	265.76	0.00
344.54	0.21	0.02
346.87	0.17	0.03
358.00	0.00	10.11
360.15	0.10	10.03
381.77	0.00	22.39
551.46	0.00	0.00
551.68	0.00	9.11
551.78	0.00	0.00
551.96	0.00	9.08
555.84	0.00	0.02
555.86	0.00	0.00
589.92	12.88	0.00
591.27	0.00	46.87
629.54	0.00	0.01
631.02	0.00	0.68
631.65	0.00	0.02
632.48	0.00	0.48
803.17	2.95	0.00
803.32	2.88	0.00
804.03	0.00	0.00
804.15	0.00	0.00
957.60	0.00	0.00
957.80	0.00	0.00
958.13	0.00	0.11
958.24	0.00	0.11

1045.45	17.97	0.00
1045.58	0.00	2.00
1046.21	17.88	0.01
1046.36	0.00	1.98
1054.83	0.23	0.00
1055.10	0.00	2.14
1055.51	0.00	0.00
1055.63	0.03	2.11
1055.83	0.12	0.00
1056.13	0.01	1.96
1081.96	1.62	0.00
1082.06	0.00	4.17
1082.20	1.61	0.00
1082.31	0.00	4.14
1123.32	0.00	0.00
1123.33	0.00	0.00
1179.49	0.00	0.01
1179.54	0.00	0.00
1180.41	0.00	2.65
1180.48	0.00	2.76
1399.95	0.00	0.00
1400.17	0.01	0.00
1400.56	0.00	0.24
1400.83	0.00	0.36
1418.63	49.69	0.00
1419.50	0.00	10.86
1419.99	0.93	5.84
1420.11	0.00	44.81
1420.38	0.47	7.09
1420.74	0.53	19.48
1420.96	0.00	1.46
1421.18	0.16	35.07

1421.64	1.09	4.59
1422.09	0.49	22.35
1443.29	6.54	0.00
1443.91	0.00	176.06
1463.39	12.40	0.00
1463.74	12.58	0.00
1464.01	0.00	8.40
1464.36	0.00	8.49
1484.22	0.01	0.46
1484.61	0.00	0.00
1486.21	0.02	1.20
1486.39	0.00	1.06
1489.71	0.00	0.06
1490.10	0.00	0.00
1493.09	0.00	49.72
1493.13	0.35	49.91
1494.64	0.03	0.02
1494.73	0.02	0.04
1505.98	58.90	0.29
1507.10	0.00	5.48
1510.93	0.00	0.02
1511.36	0.01	0.00
1511.79	0.00	43.90
1512.09	0.00	44.74
1517.29	26.20	0.01
1517.40	25.50	0.00
1517.61	0.00	12.73
1517.72	0.00	12.71
3017.65	0.04	0.03
3017.70	0.04	135.80
3017.80	0.00	17.29
3017.86	9.10	130.51

3018.31	0.02	368.32
3018.33	0.00	353.26
3018.46	243.80	0.20
3018.47	235.32	5.01
3020.42	203.90	0.04
3021.34	0.01	2009.55
3079.03	0.06	0.64
3079.26	0.00	13.60
3079.29	0.08	15.11
3079.56	1.49	12.15
3079.62	0.06	159.18
3079.91	0.00	146.14
3080.06	24.64	0.66
3080.35	25.42	1.02
3081.45	85.98	0.10
3081.89	0.01	378.56
3108.56	0.00	0.21
3108.70	0.81	0.00
3111.34	0.01	21.79
3111.54	0.00	20.48
3111.64	105.80	0.08
3111.83	101.79	1.14
3114.10	0.00	0.16
3114.17	0.00	0.00
3114.33	0.83	155.37
3114.44	0.01	154.81

Table S5: Calculated structural parameters (Å) of ZnCp*₂ (Gaussian 03):

No.	Atom	x	y	z
1	Zn	0.418	-0.014	-0.315
2	H	-3.566	-1.304	2.301
3	C	1.010	0.101	3.003
4	C	1.595	0.047	1.618
5	C	2.001	1.178	0.832
6	C	1.848	-2.550	1.425
7	C	1.899	2.620	1.247
8	C	2.630	0.687	-0.359
9	C	3.298	1.526	-1.413
10	C	2.613	-0.746	-0.312
11	C	3.263	-1.667	-1.307
12	C	1.976	-1.143	0.910
13	C	-3.764	1.561	1.238
14	C	-2.915	0.737	0.313
15	C	-2.923	-0.726	0.318
16	C	-1.771	2.589	-1.073
17	C	-3.781	-1.535	1.248
18	C	-2.040	-1.182	-0.623
19	C	-1.798	-2.601	-1.055
20	C	-1.370	-0.008	-1.257
21	C	-1.241	-0.014	-2.783
22	C	-2.028	1.177	-0.631
23	H	3.282	1.040	-2.394
24	H	4.352	1.711	-1.163
25	H	2.819	2.503	-1.523
26	H	1.831	3.289	0.384
27	H	2.779	2.929	1.828
28	H	1.019	2.802	1.873
29	H	0.382	-0.769	3.214

30	H	0.393	0.993	3.150
31	H	1.801	0.124	3.765
32	H	1.755	-3.276	0.612
33	H	0.975	-2.669	2.073
34	H	2.731	-2.837	2.014
35	H	2.771	-2.644	-1.342
36	H	4.317	-1.846	-1.053
37	H	3.243	-1.253	-2.321
38	H	-3.603	2.633	1.094
39	H	-3.552	1.334	2.292
40	H	-4.833	1.366	1.084
41	H	-2.206	2.786	-2.064
42	H	-0.699	2.811	-1.151
43	H	-2.204	3.317	-0.381
44	H	-0.713	-0.901	-3.149
45	H	-0.704	0.865	-3.154
46	H	-2.239	-0.011	-3.245
47	H	-2.241	-3.319	-0.359
48	H	-0.728	-2.835	-1.128
49	H	-2.232	-2.799	-2.046
50	H	-3.634	-2.610	1.110
51	H	-4.848	-1.328	1.093

Comment [A1]:

Table S6: Vibrational spectrum of ZnCp*₂ (Gaussian 03):

ν (cm ⁻¹)	IR intensity (km/mole)	Raman intensity (Å ⁴ /amu)
11.18	0.10	0.54
14.13	0.14	0.52
24.88	0.34	0.27
56.38	0.10	2.05
83.94	0.09	6.57
85.37	0.90	5.98
92.08	0.66	0.57
96.79	0.91	0.36
98.38	0.18	0.72
103.43	0.37	1.02
109.37	0.03	1.32
114.33	0.00	0.58
119.72	0.01	4.62
125.03	0.00	0.69
127.36	0.01	0.27
141.34	0.36	0.04
147.53	0.01	0.01
148.93	0.01	0.01
155.77	0.00	0.05
159.76	1.53	1.05
169.34	0.48	0.54
191.32	6.77	0.46
225.91	0.21	0.26
249.41	1.47	3.40
259.86	0.28	0.07
269.77	4.02	1.01
280.58	1.04	0.38
281.07	1.09	0.23

288.44	0.02	0.30
291.29	0.03	0.27
294.09	1.09	0.66
307.12	0.22	0.61
338.80	65.47	13.76
346.99	0.45	5.64
355.83	32.98	7.33
372.71	0.05	1.93
437.31	25.99	4.08
526.24	0.73	3.05
546.07	0.27	3.59
551.28	0.00	4.82
551.77	0.00	4.73
554.53	0.00	0.01
568.16	0.58	0.61
589.27	6.49	19.17
598.47	3.42	22.84
632.31	0.04	0.29
633.76	0.05	0.32
671.47	0.52	0.18
707.29	15.35	48.85
797.06	1.68	0.28
800.88	0.72	0.03
801.68	1.19	0.07
815.27	4.44	33.96
955.32	13.64	5.95
956.95	1.02	0.65
957.36	0.76	0.45
958.19	0.11	0.12
1034.44	0.84	0.26
1043.16	2.59	0.40
1045.47	8.98	0.84

1046.29	9.18	0.79
1054.75	0.06	1.19
1055.42	0.08	0.99
1056.29	0.10	0.87
1057.55	0.36	3.20
1065.37	2.19	2.78
1068.94	1.75	0.10
1075.52	7.87	45.39
1078.72	0.13	0.28
1080.90	0.81	1.67
1081.67	1.03	2.23
1117.42	1.27	0.36
1122.77	0.00	0.00
1153.14	4.50	3.58
1154.04	0.91	1.21
1179.94	0.01	1.41
1180.28	0.00	1.25
1274.49	46.11	1.90
1330.94	0.35	0.11
1377.36	0.46	15.50
1400.13	0.10	0.11
1401.04	0.03	0.09
1409.73	3.80	4.58
1411.14	0.97	12.44
1416.74	1.94	33.80
1418.57	11.99	12.71
1419.97	0.35	9.57
1420.05	0.30	15.97
1420.75	0.52	21.75
1421.50	2.32	5.02
1422.47	3.21	3.17
1430.23	0.95	22.75

1442.06	2.13	79.09
1461.88	7.20	3.45
1462.34	7.88	1.82
1481.03	0.54	0.22
1482.67	1.70	3.62
1482.96	0.11	11.73
1485.17	9.09	12.19
1485.56	4.27	17.42
1488.46	2.87	8.96
1489.08	3.56	6.60
1490.15	0.48	1.53
1491.66	1.16	12.05
1492.66	1.14	17.83
1494.17	19.82	8.91
1495.27	3.33	14.63
1501.49	0.52	44.50
1503.53	8.88	4.86
1504.44	23.51	10.11
1505.60	4.74	1.98
1511.63	0.17	21.08
1512.43	0.42	22.31
1516.61	11.43	3.71
1517.21	11.34	4.13
1584.82	4.98	85.16
1651.57	6.25	2.35
3005.31	52.33	136.97
3010.10	69.20	88.24
3011.52	71.54	331.71
3016.97	13.36	19.83
3019.36	0.78	60.10
3019.53	7.61	71.86
3019.94	100.99	173.04

3020.10	107.04	157.38
3020.59	134.79	277.87
3022.51	60.38	1385.80
3055.75	13.57	64.08
3056.60	42.52	75.68
3059.06	0.65	0.26
3061.33	47.40	211.69
3078.72	20.57	62.76
3079.92	1.47	15.38
3080.36	9.00	62.23
3081.40	16.48	95.83
3082.29	16.67	67.49
3084.64	28.83	102.30
3106.27	23.50	9.43
3109.37	6.41	2.98
3109.53	8.31	49.98
3109.71	20.37	32.03
3112.08	48.97	22.43
3113.22	37.40	28.73
3114.70	4.83	71.13
3117.39	1.97	44.21
3118.40	69.19	39.64
3119.34	1.43	138.96