Supporting Information File for

Conformational Analysis and Vibrational Circular Dichroism of tris(ethylenediamine)ruthenium(II) Complex : A Theoretical Study

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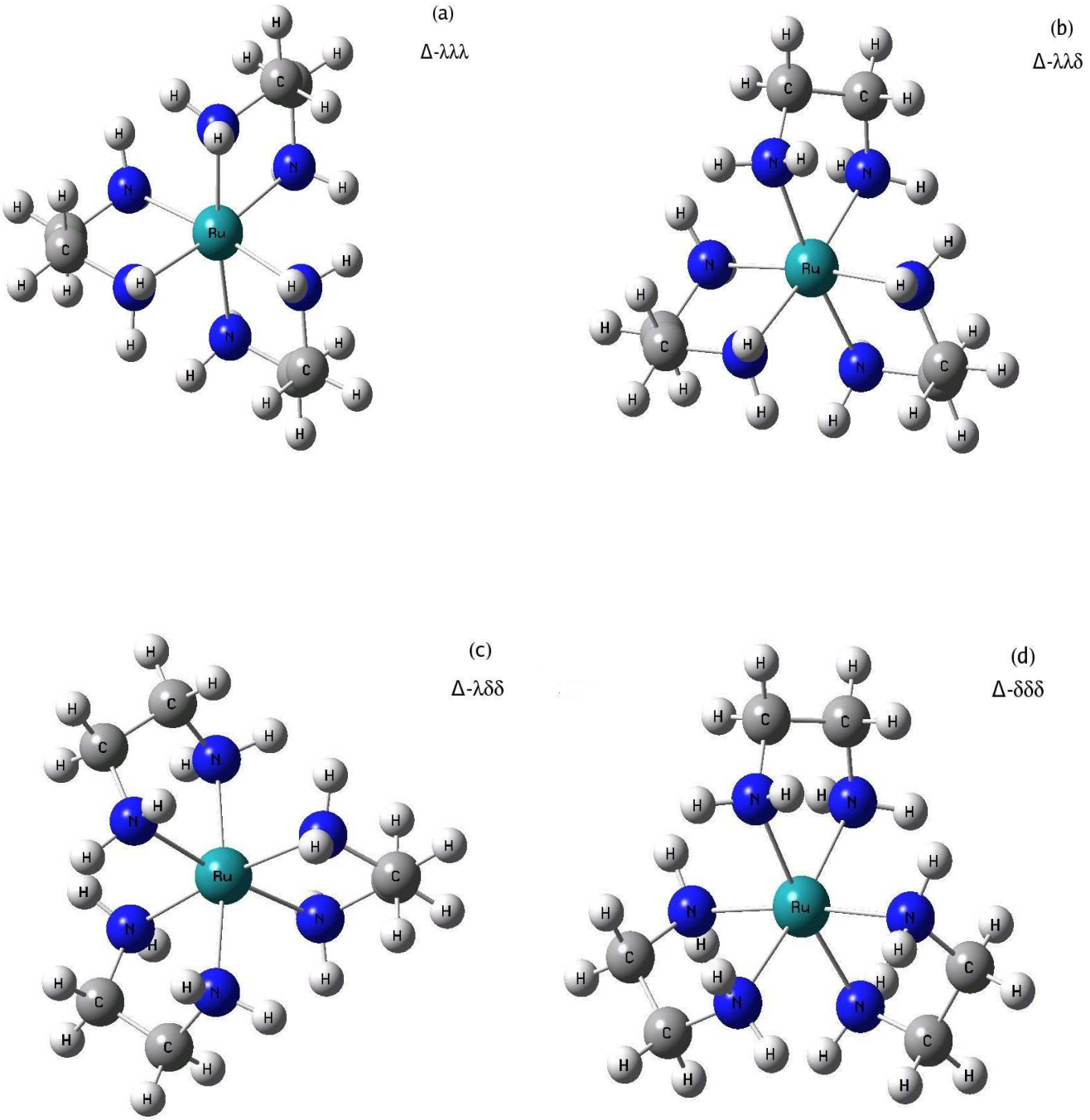

Figure S1. The Optimized geometries for the four conformers (λλλ), (λλδ), (λδδ) and (δδδ) of Δ–$[Ru(en)_3]^{2+}$.

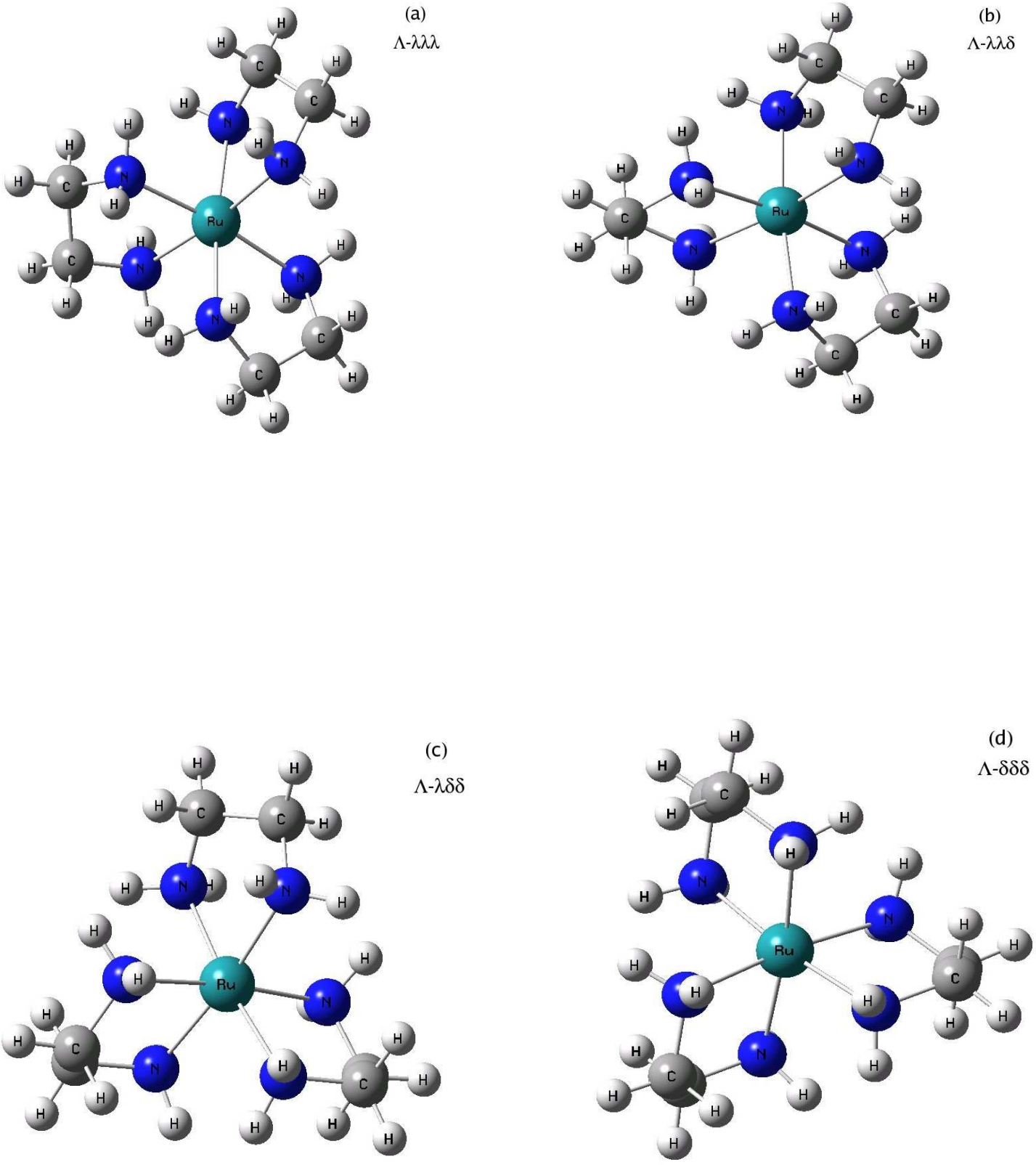

Figure S2. The optimized geometries for the four conformers (λλλ), (λλδ), (λδδ) and (δδδ) of Λ–$[Ru(en)_3]^{2+}$.

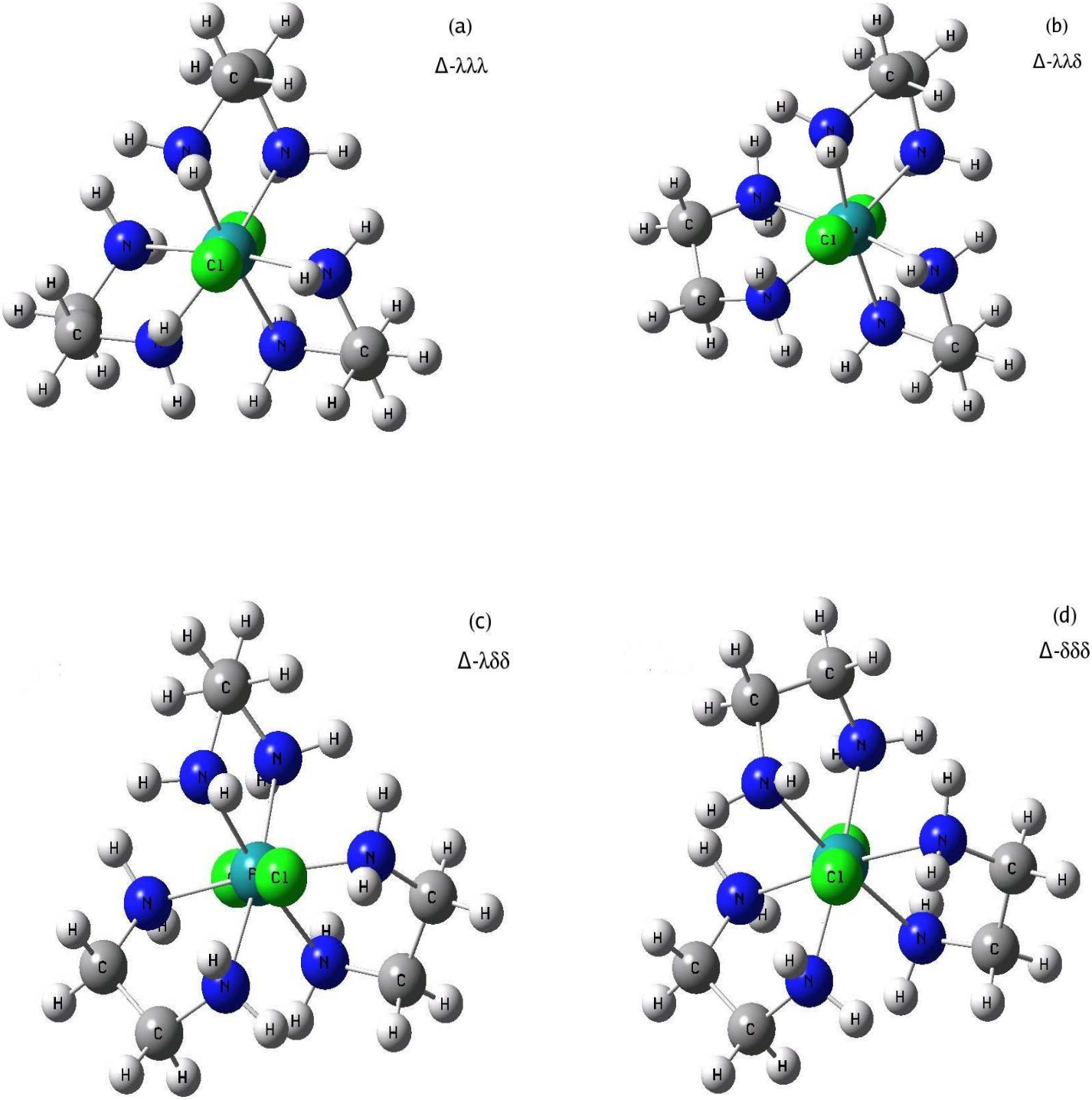

Figure S3. Optimized geometries for the four conformers (λλλ) , (λλδ), (λδδ) and (δδδ) of Δ–[Ru(en)$_3$] Cl_2.

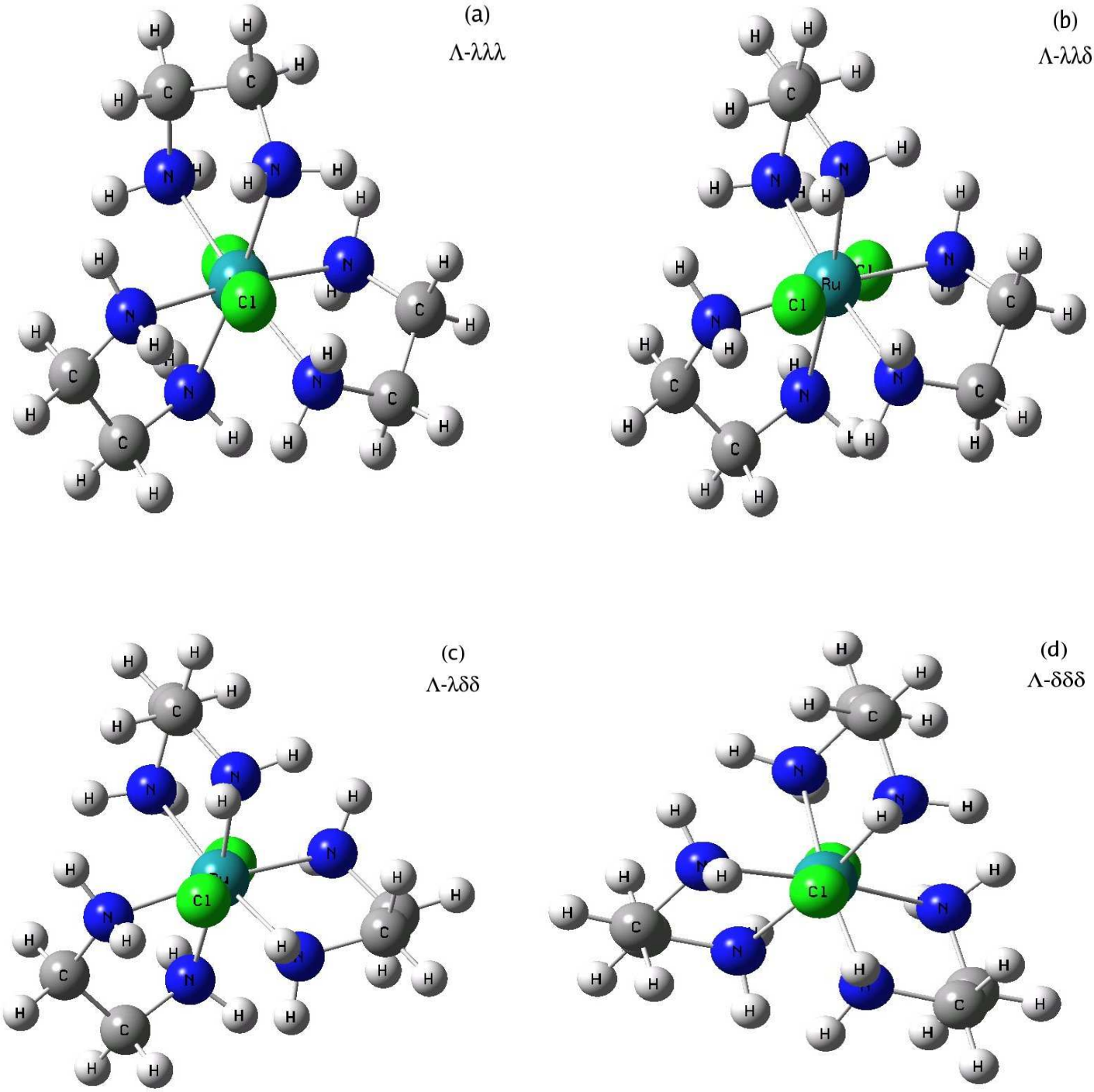

Figure S4. Optimized geometries of the four conformers (λλλ), (λλδ), (λδδ) and (δδδ) of Λ-[Ru(en)3]Cl_2.

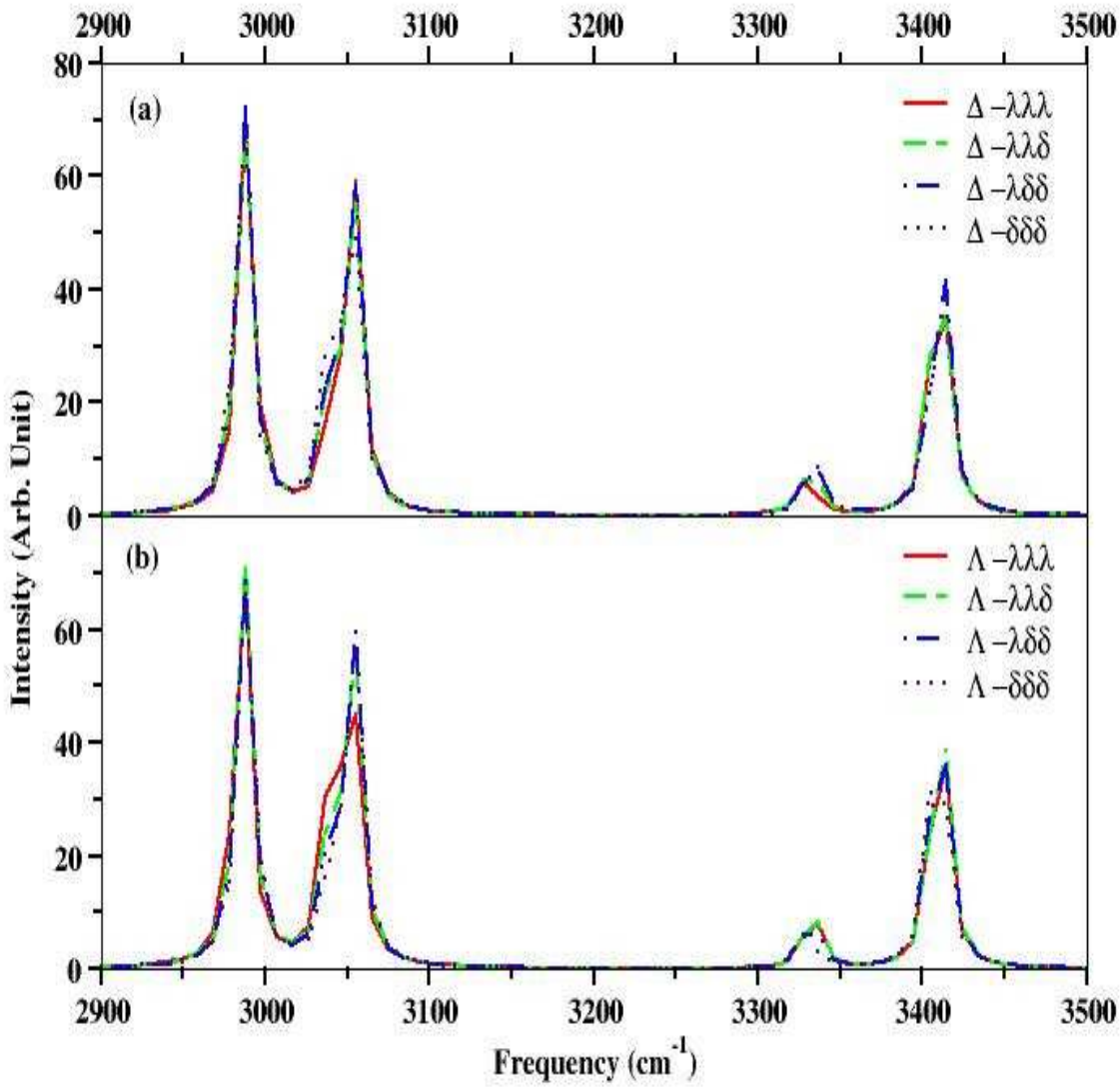

Figure S5. IR absorbance spectra for CH and NH- stretching modes for (a) the four conformers of Δ-$[Ru(en)_3]^{2+}$ and (b) the four conformers of Λ-$[Ru(en)_3]^{2+}$. Scale factor is 0.97.

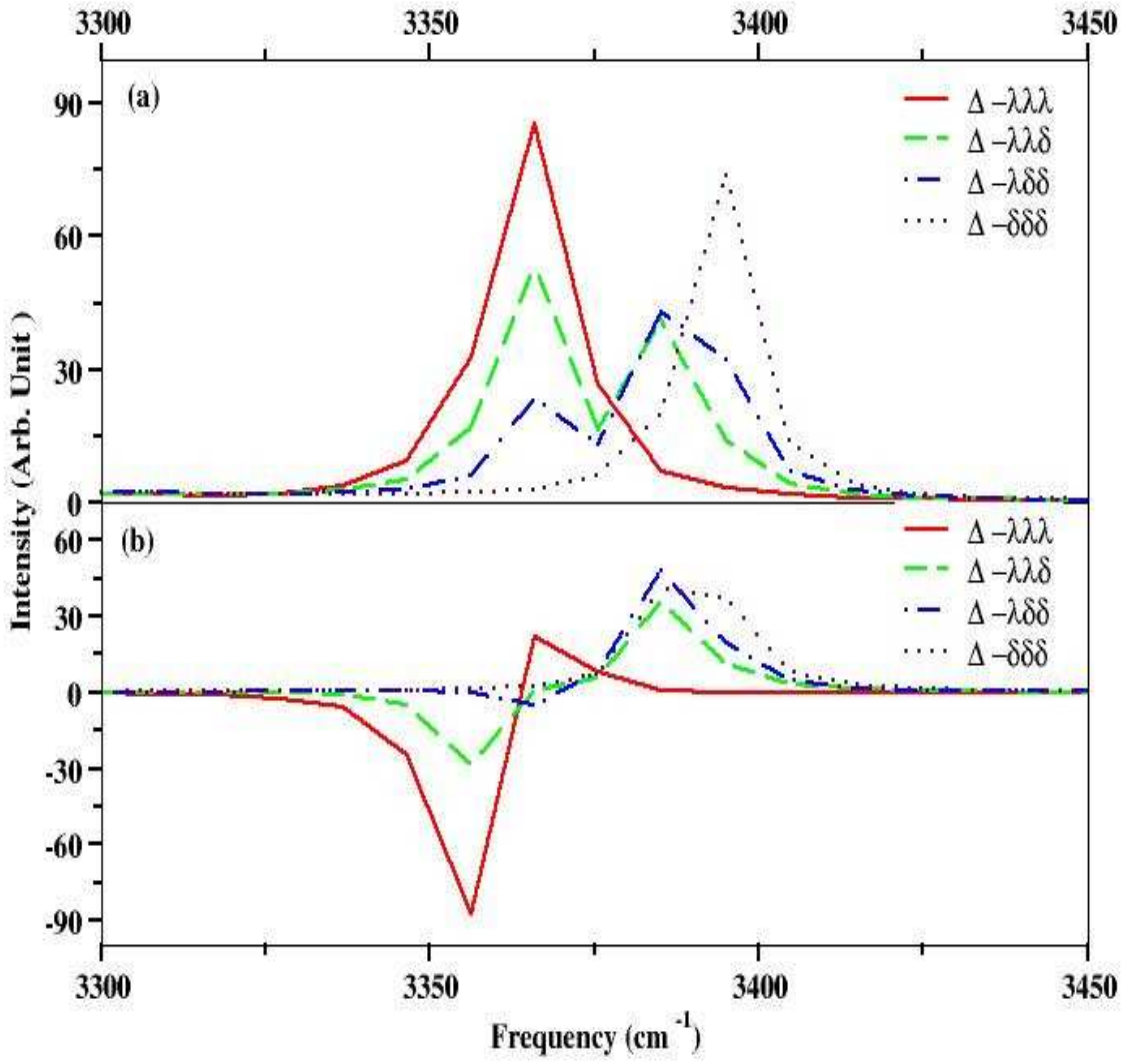

Figure S6. (a) Absorbance and (b) VCD spectra generated by NH -antisymmetric stretches for all the four conformers of the association complex, Δ -$[Ru(en)_3]$ Cl_2.

Table S1: Optimized bond lengths (Angstroms) and bond angles (Degrees) of Δ-tris(ethlyenediamine) ruthenium(II)chloride, Δ-$[Ru(en)_3]Cl_2$.

Variable	Δ(λλλ)	Δ(λλδ)	Δ(λδδ)	Δ(δδδ)
Bond Length (A˚)				
Ru (37)- Cl(38)	3.80	3.78	3.76	3.71
Ru(37)-N(1)	2.17	2.17	2.17	2.18
N(1)-C(18)	1.50	1.50	1.50	1.50
C(18)-C(21)	1.54	1.54	1.54	1.54
C(24)-C(34)	1.54	1.54	1.54	1.54
N(1)-H(3)	1.02	1.02	1.02	1.02
Bond Angles (deg.)				
N(12)-Ru(37)-N(15)	93.37	93.12	92.95	95.21
Ru(37)-N(1)-C(18)	107.83	107.64	108.14	109.10
N(1)-Ru(37)-N(9)	82.08	81.99	81.95	81.62
C(24)-N(15)-H(17)	110.134	110.10	110.16	109.79
N(15)-C(24)-C(34)	109.57	109.51	109.55	110.57
N(12)-C(24)-C(34)	109.46	109.46	109.55	110.58
Dihedral angles Dω (deg.)				
N(1)-C(18)-C(21)-N(9)	-54.83	-54.57	-54.11	49.54
N(15)-C(24)-C(34)-N(12)	-54.44	-54.57	49.61	49.31
N(4)-C(38)-C(28)-N(6)	-54.43	50.86	49.611	49.07

Table S2: Relative conformational energy changes along the conformational pathways between different conformational isomers of Δ-$[Ru(en)_3]^{2+}$

S.NO	Dihedral angle (deg.) D_ω	Relative angle change(deg.)	Single point energy E(RB+HF-LYP) (a.u)	Relative conformational energy (Kcal/mol)
Δ(λλλ)	D_ω of 1st ring (λλλ)	(-60.00=0.00)		
1.	-55.09	4.91	-665.02677647	0.204
2.	-35.24	24.76	-665.02026950	4.287
3.	-15.16	44.84	-665.01288392	8.922
4.	-0.32	59.68	-665.01182021	9.589
5.	14.54	74.54	-665.01262887	9.082
6.	35.80	95.80	-665.01862643	5.318
7.	54.56	114.56	-665.02693875	0.102
Δ(λλδ)	D_ω of 2nd ring (λλδ)	(-54.83=114.56)		
8.	-54.83	114.56	-665.02693875	0.102
9.	-34.87	134.52	-665.02003469	4.434
10	-14.87	154.52	-665.01255895	9.125
11.	- 0.45	168.94	-665.00803751	11.963
12.	14.07	183.46	-665.0120509	9.444
13.	33.97	203.36	-665.01885199	5.177
14	54.36	223.75	-665.02704780	0.034
Δ(λδδ)	D_ω of 3rd ring (λδδ)	(-54.92=223.75		
15.	-54.92	223.75	-665.02704780	0.034
16.	-37.92	240.75	-665.02283791	2.675
17.	-15.96	262.71	-665.01315720	8.750

S.NO	Dihedral angle (deg.) D_{ω}	Relative angle change(deg.)	Single point energy E(RB+HF-LYP) (a.u)	Relative conformational energy (Kcal/mol)
18.	0.40	279.07	-665.01111796	10.030
19.	15.48	293.40	-665.01266804	9.057
20.	34.56	313.23	-665.01957183	4.725
21.	54.92	333.59	-665.02710131	0.000

Table S3 : Relative conformational energy changes along the conformational pathways between different conformational isomers of Δ–[$Ru(en)_3$]Cl_2 .

S.NO	Dihedral angle (deg.) D_ω	Relative angle change(deg.)	Single point energy E(RB+HF-LYP) (a.u)	Relative conformational energy (Kcal/mol)
Δ(λλλ)	Dω of 1st ring (λλλ)	(-60.00=0.00)		
1.	-54.43	5.57	-695.51740633	0.00
2.	-35.88	24.12	-695.51107546	3.973
3.	-15.47	44.53	-695.50204872	9.637
4.	-0.05	59.95	-695.49834102	11.964
5.	15.85	75.85	-695.50085505	10.386
6.	35.24	95.24	-695.50593199	7.200
7.	50.86	110.86	-695.51111627	3.947
Δ(λλδ)	D_ω of 2nd ring (λλδ)	(-54.57=110.86)		
8.	-54.57	110.86	-695.51111627	3.947
9.	-34.98	130.45	-695.50530427	7.594
10	-15.02	150.41	-695.49596261	13.456
11.	0.72	166.15	-695.49339048	15.070
12.	15.14	180.57	-695.49374322	14.849
13.	35.32	200.75	-695.49810986	12.109
14	49.61	215.04	-695.50465103	8.004
Δ(λδδ)	D_ω of 3rd ring(λλλ)	(-54.11=215.04)		
15.	-54.11	215.04	-695.50465103	8.004
16.	-35.48	233.67	-695.49881769	11.665
17.	-15.42	253.73	-695.49020391	17.070
18.	0.15	269.3	-695.47762302	24.964
19.	15.63	284.78	-695.48689486	19.146
20.	35.26	304.41	-695.49183206	16.048
21.	49.54	318.69	-695.49781301	12.295

Table S4: Frequency (cm^{-1}) assignment of the $[Ru(en)_3]^{2+}$ complex. Be bending, Ro rocking, Tw twisting, Sc scissoring, Str stretching, Wa wagging. All frequencies are scaled by a factor of 0.97.

S.NO	Assignment	Δ-$[Ru(en)_3]^{2+}$				Λ-$[Ru(en)_3]^{2+}$			
		Δ(λλλ)	Δ(λλδ)	Δ(λδδ)	Δ(δδδ)	Λ(λλλ)	Λ(λλδ)	Λ(λδδ)	Λ(δδδ)
1	N-C-C-N, Wa	66.6	66.1	72.8	69.4	70.3	75.7	67.4	58.1
2	N-C-C-N, Wa	75.4	79.4	75.5	74.2	73.7	79.4	77.2	68.5
3	Ru-N2Wa,Ro	82.9	85.3	95.7	100.5	99.6	98.2	85.8	82.5
4	Ru-N2,Tw	121.7	122.2	120.2	117.5	118.3	118	121.2	121.6
5	Ru-N2, Tw	124.8	126.7	122.3	119.9	121.3	123.7	127.1	124.2
6	Ru-N2, Tw	145.5	137.7	133.1	132	132	132.5	138.2	142
7	Ru-N2, Wa,	184.2	180.7	178.8	176.4	177.6	177.7	179.6	183.2
8	Ru-N2, Wa,	189.2	186.8	184.3	179.6	181.3	183.1	187.8	186.5
9	Ru-N2, Wa,	202.2	196.2	188.9	188.5	188.2	190.6	195.4	199.5
10	Ru-N2, sym.Str	223.7	219.9	217.1	215.3	215.3	217.6	219.6	222.8
11	N -C-C, Be ; CH2 ,Ro	261.9	264.7	273.4	274.4	274.5	270.7	264.3	260.2
12	N -C-C, Be ; CH2 ,Ro	267.2	271.2	277.9	276.7	276.1	277.3	271.6	263
13	N -C-C, Be ; CH2 ,Ro	289.7	278.1	283.5	281.6	282.1	284.6	277.3	286.8
14	Ru-N2, sym Str	298.5	297.7	294.1	293.2	293.3	293	296.9	296.7
15	Ru-N2, sym Str	303.3	298.8	298.8	295.9	296	300.1	299	301.8
16	Ru-N2, antisym Str	348	348.5	349.1	347.4	348.3	348.2	348.6	348.5
17	Ru-N2 , antisym Str	351.7	351.3	350.8	350.1	349.5	349.7	351.5	352.8
18	Ru-N2, antisym Str	356.9	358.3	352.3	353.6	355.2	354.7	356.8	354.8
19	Ru-N2, Sc	405.1	405.6	404.7	406.2	407.2	404.5	405.2	405.6
20	Ru-N2, Sc	408.1	410.5	408.2	408.7	408.3	410	410.6	406.9
21	Ru-N2 , Sc	439.6	438.3	437.4	436.6	436.8	437	438.3	439.3
22	CH2+NH2 , Ro	490.2	499	502.7	501.8	502.7	503.8	499	488.4
23	CH2+NH2 , Ro	524.6	509.4	507.8	505.4	505.3	508.5	509	523.4
24	CH2+NH2 , Ro	529.4	526.5	523.4	533.2	533.5	523.3	526.6	528
25	NH2, Ro	591.8	601.3	608.9	610.7	611.8	605.4	602	592.5
26	NH2, Ro	594.8	610.6	614.3	626.6	626.2	618.1	610.8	596.3
27	NH2, Ro	661.3	656.6	650.5	629.2	629.4	648.4	656.7	660.4
28	NH2+CH2, Ro	682.7	670.4	651.9	647.3	647.9	652	669.7	682.5
29	NH2+CH2, Ro	685.3	678.9	682.6	706.3	705.9	684	679	686.2
30	NH2+CH2, Ro	697.9	701.1	707.6	709.1	709.7	707.7	702.3	697.2
31	NC +CC Str	841.7	841	841	840.3	840.3	841	840.9	841.6
32	NC +CC Str	841.9	841.4	841.7	841.1	841	841.2	841.2	842
33	NC +CC Str	842.9	842.5	842.5	842.7	842.6	842.4	842.1	842.9
34	NC +CC Str	845.5	843	843.5	842.8	842.7	843.6	843.2	845.5
35	NC +CC Str	848.2	846.7	847.1	843.4	843.4	847.2	846.4	847.7
36	NC +CC Str	849.1	848	850.7	853	853	851	847.7	848.1
37	CH2,Ro;, NH2,Tw	950.7	952.4	954.9	954.6	955.3	954.8	952.8	951.5
38	CH2,Ro ; NH2,Tw	955.4	953.6	955.2	955.9	956.1	955.5	953.5	953.8
39	CH2, Ro ;,NH2,Tw	966.2	962.7	960.9	958.8	959	960.2	962.9	965.3
40	N-C ,Str	981.8	980.8	980.2	980.5	980.3	980.5	980.1	981.1
41	N-C ,Str	982.7	981.8	982	982.5	982.1	982	981.7	982.3
42	N-C ,Str	983.1	982.2	983.1	982.8	983	983.9	982.1	982.5

43	N-C ,Str	1021.9	1021.1	1022.3	1022.9	1023.1	1022.6	1021.9	1021.8
44	N-C+C-C, Str	1022.1	1023.8	1022.6	1024.1	1024.2	1023.1	1023.6	1022.7
45	N-C+C-C, Str	1035.4	1033.1	1031.3	1031.1	1031.2	1031.7	1033.5	1035.7
46	NH2+CH2, Tw	1065.7	1068.9	1067.3	1065.1	1066.2	1066.6	1068.6	1065.9
47	NH2+CH2,Tw	1077.8	1071.3	1074.4	1066.6	1067.1	1074.2	1071.5	1077.6
48	NH2+CH2,Tw	1080.1	1078.6	1077.9	1080	1080.5	1077.6	1079.7	1080.1
49	NH2, Wa ; N-C-H, Be	1124.6	1122.4	1121.1	1121.4	1122.1	1120.9	1122.5	1124.7
50	NH2,Wa ; N-C-H, Be	1124.8	1125.7	1123.6	1122.8	1123.1	1124.6	1125.9	1125.8
51	NH2,Wa ; N-C-H, Be	1140.9	1137.5	1133.1	1136.6	1137	1133.4	1138.2	1141.2
52	NH2,Wa,	1151.1	1147.9	1146.3	1145.6	1145.8	1145.8	1148.1	1151.3
53	NH2,Wa,	1152.8	1150.2	1148.8	1146.9	1147	1149.5	1151.4	1153.9
54	NH2 ,Wa	1166.7	1166.3	1165.4	1170.4	1170.6	1165.6	1166.7	1167.7
55	NH2+CH2,Tw	1263.7	1261.8	1262.2	1261.7	1262	1262.2	1261.6	1263.6
56	NH2+CH2,Tw	1264.5	1264.4	1264.7	1262.5	1262.9	1264.7	1264.7	1264.1
57	NH2+CH2,Tw	1266.9	1266.9	1267.8	1267.4	1267.6	1267.4	1267.3	1267.1
58	CH2, Tw; NH2, Wa	1284.2	1282.8	1283	1282.1	1282.4	1282.9	1283.1	1284
59	CH2,Tw ; NH2, Wa	1284.5	1285.8	1285	1283.3	1283.5	1285.4	1285.3	1284.6
60	CH2,Tw ; NH2, Wa	1291.1	1287.6	1287.6	1288.5	1288.7	1287.4	1288.1	1290.9
61	CH2 +NH2, Tw	1311.9	1311.3	1312.1	1311.4	1311.7	1311.8	1311.7	1312
62	CH2 +NH2, Tw	1313.5	1313.2	1313	1311.6	1311.8	1313	1313.1	1313
63	CH2 +NH2, Tw	1314.5	1314.6	1315.4	1315.3	1315.4	1315.1	1314.8	1314
64	CH2, Wa ; NH2 Tw	1375.3	1374.9	1375.6	1375.3	1375.5	1375.4	1375.2	1375.4
65	CH2,Wa ; NH2 Tw	1375.8	1375.4	1376.6	1376	1376.1	1376.8	1375.6	1375.9
66	CH2,Wa ; NH2 Tw	1376.4	1376.6	1377.5	1377.8	1377.9	1377.7	1376.4	1376.3
67	CH2,Wa ; NH2 Tw	1395	1394.5	1394.4	1393.9	1394.2	1394.1	1394.8	1394.8
68	CH2, Wa ; NH2 Tw	1395.6	1395.6	1396.4	1395	1395.1	1396.9	1395.7	1395.6
69	CH2,Wa ; NH2 Tw	1397.9	1396.8	1397	1397.7	1397.9	1397.5	1396.9	1398.1
70	CH2, Sc	1473.6	1474.8	1476.4	1476.9	1476.7	1476.3	1475.6	1473.7
71	CH2,Sc	1476.5	1476	1477.1	1478	1478.3	1477.3	1475.9	1475.5
72	CH2,Sc	1478.9	1478.1	1479.9	1479.1	1479.1	1478.2	1477.4	1476.6
73	CH2,Sc	1479	1479	1482	1482.3	1482.3	1481.3	1478.9	1478.1
74	CH2,Sc	1482	1481.2	1483.1	1483.1	1482.7	1483.2	1481	1479.9
75	CH2,Sc	1483.3	1481.9	1485	1483.5	1483.4	1487.1	1481.5	1484.8
76	NH2,Sc	1641.5	1638.7	1639.8	1646.7	1646.7	1639.6	1638.6	1641.8
77	NH2, Sc	1651.7	1652.2	1649.8	1652.4	1652.5	1649.7	1652	1651.7
78	NH2, Sc	1653.5	1652.6	1654	1654.6	1655	1653.5	1653.1	1654
79	NH2, Sc	1654.1	1654.7	1659.5	1658.4	1658.5	1658.5	1654.5	1654.8
80	NH2, Sc	1660.7	1662.5	1663.6	1661.3	1661.2	1663	1662.2	1661.3
81	NH2,Sc	1661.8	1667.5	1667.6	1662.9	1663.7	1667.7	1667.7	1661.8
82	CH2,sym Str	2986.5	2985.1	2985.4	2984.2	2984.1	2985.1	2985.5	2986.3
83	CH2,sym Str	2986.9	2985.7	2985.9	2985.3	2984.8	2986.2	2986	2986.5
84	CH2,sym Str	2987.2	2986.2	2987.2	2985.9	2985.4	2986.3	2986.3	2987.7
85	CH2,sym Str	2989.9	2988.5	2988.2	2986.5	2986.2	2987.8	2989.3	2989.4
86	CH2,sym Str	2990.3	2989.3	2988.6	2988.2	2988.1	2989.5	2989.8	2989.6
87	CH2,sym Str	2990.7	2990.4	2990.8	2989.2	2988.2	2989.9	2990.6	2991.9
88	CH2, antisym Str	3041.4	3039.8	3039.7	3038.2	3038.3	3039.5	3040.2	3041.4
89	CH2, antisym Str	3041.9	3040.7	3039.9	3039.3	3039	3040.1	3040.6	3041.7
90	CH2, antisym Str	3042	3040.9	3041.4	3039.7	3039.3	3040.2	3040.9	3042.4
91	CH2, antisym Str	3054.6	3053	3052.9	3051.2	3051	3052.5	3053.7	3054.4
92	CH2, antisym Str	3055.3	3053.9	3053.2	3052.5	3052.2	3053.8	3054.2	3054.8
93	CH2, antisym Str	3055.4	3054.7	3055.2	3053.4	3052.5	3053.9	3054.9	3056.2
94	NH2, sym Str	3322	3324.3	3329.1	3332.1	3331.7	3329.1	3323.9	3321.9
95	NH2, sym Str	3323.2	3327.4	3329.4	3332.8	3332.1	3329.8	3327.6	3322.8

96	NH2, sym Str	3323.8	3329.1	3332.6	3334.6	3334.1	3332.2	3329.8	3323.2
97	NH2, sym Str	3329.2	3330.6	3333.2	3335.5	3334.7	3333.9	3330.4	3329
98	NH2, sym Str	3330.2	3332	3337.9	3335.8	3335.4	3336.6	3333.3	3329.8
99	NH2,sym Str	3332.2	3337	3338	3336.3	3336.2	3336.9	3338	3332.2
100	NH2, antisym Str	3406.9	3407.1	3409.4	3409.6	3409.3	3408.5	3407	3406.3
101	NH2, antisym Str	3407.5	3407.5	3409.5	3410.4	3409.6	3409.3	3408.2	3406.6
102	NH2, antisym Str	3408.5	3409.1	3410.4	3410.8	3410.3	3410	3409	3407
103	NH2, antisym Str	3410.3	3409.6	3410.8	3411.3	3410.8	3411.1	3410.3	3410.1
104	NH2, antisym Str	3411.4	3411.3	3413.1	3412	3411.4	3412.3	3411	3410.5
105	NH2, antisym Str	3411.9	3412.8	3413.8	3413	3412.7	3412.9	3414.1	3410.8

Table S5: Frequency (cm^{-1}) assignment of the $[Ru(en)_3]Cl_2$ complex. Be bending, Ro rocking, Tw twisting, Sc scissoring, Str stretching, Wa wagging. All frequencies are scaled by a factor of 0.97.

S.NO	Assignment	Δ-$[Ru(en)_3]Cl_2$				Λ-$[Ru(en)_3]Cl_2$			
		Δ(λλλ)	Δ(λλδ)	Δ(λδδ)	Δ(δδδ)	Λ(λλλ)	Λ(λλδ)	Λ(λδδ)	Λ(δδδ)
1	RuCl2,Be; NCCN,Wa	69.3	70.2	57.8	62.9	66.3	58.9	70.2	71
2	RuCl2,Be; NCCN,Wa	76.2	76.5	63.1	72.1	71	65.5	76.5	73.8
3	RuCl2,Be; RuN2,Wa	82.3	81.7	68.7	73.6	72.3	68.9	81.8	82.1
4	RuCl2,Be; RuN2,Wa	90.2	86.7	78.2	84.2	75.1	78.2	86.7	86.6
5	Ru-N2, Wa	106.8	107.1	106.4	106.2	104.5	106.5	107.1	106.3
6	Ru-N2, Ro	115.4	111.9	108.3	110	106.8	108.7	112	115.8
7	Ru-N2, Ro	117.8	115.2	114.7	119.3	111.5	115.3	115.1	118.1
8	Ru-Cl2, Str; RuN2,Tw	128.2	122	121.3	123.7	121.8	121.4	122.1	126.8
9	Ru-Cl2,Str; RuN2,Tw	168.7	164.6	152.6	153.4	155.4	153.3	164.6	168.1
10	Ru-Cl2,Str; RuN2,Tw	169.7	166.5	165.9	158.3	156.8	165.6	166.5	169.4
11	RuCl2,Be; RuN2,Tw	171.1	169.3	166.5	164.3	163.3	167	169.3	170.3
12	RuCl2,Str; RuN2,Tw	194.2	188.5	183.7	187.1	182.3	184.1	188.5	194.3
13	RuN2, Wa	226.6	216.6	203.3	208.4	200.4	203.1	216.5	226.7
14	RuN2,Wa	230.2	218	210	210.7	205	210.6	218	230.6
15	Ru-N2, sym Str	239.7	240.8	236.1	227.6	225.8	236.2	240.8	238.8
16	Ru-N2, sym Str	264	252.5	240.4	240.8	239.8	240.4	252.4	264.6
17	Ru-N2 Tw	270.8	270.8	258.4	261.3	261.3	257.7	270.7	269
18	Ru-N2, Str,RuN2,Tw	274.9	274.7	263.1	273.8	265.8	264.7	274.7	271.3
19	Ru-N2, Str; RuN2,Tw	323.1	292.3	287.2	275.2	270	287.3	292.3	322.9
20	Ru-N2,Str;	325.1	321.3	301.3	303.2	303.4	301.7	321.3	324.4
21	Ru-N2, Str	328.3	322.8	322	303.8	304.6	322.1	322.8	325.6
22	Ru-N2, antisym Str	375.5	375.4	375.7	371.2	376.6	375.8	375.5	374
23	Ru-N2, antisym Str	380.9	382.7	377.4	373.5	378.6	377.4	382.8	378.8
24	Ru-N2, antisym Str	385.9	383.2	380.6	379.3	381.2	381	383	384.3
25	Ru-N2, Sc	429.2	427.4	432.1	437.1	440.5	432	427.4	427.1
26	Ru-N2,Sc	433	434.6	441.4	437.8	442	441.6	434.6	430.6
27	Ru-N2,Sc	460.3	461.2	465.9	464.5	468.9	466	461.3	458.2
28	CH2+NH2 , Ro	512.2	515.5	528.8	529.5	531.7	528.8	515.5	510.7
29	CH2+NH2, Ro	536.8	539.1	531.9	535.3	533.4	532.4	539.2	536.6
30	CH2+NH2, Ro	541.4	539.6	542.1	551.1	552.6	542.6	539.6	538.6
31	NH2, Ro	681.5	661.3	653.1	638	637.8	653.5	661.3	679.6
32	NH2, Ro	683.6	685.2	667.1	658.3	659.2	666.5	685.1	681.6
33	NH2 +CH2, Ro	739.8	698.6	671.3	665.7	663.1	671.8	698.6	739
34	NH2 +CH2, Ro	747.4	721.2	712.2	695.3	689.6	712.4	721.3	746.1
35	NH2 +CH2, Ro	763	744.7	738.2	731.6	729.3	738	744.6	763.3
36	NH2 +CH2, Ro	769.6	752.8	756.8	735.9	732.8	756.7	752.9	766.1
37	NC+CC, Str	850.2	848.7	847.3	847.7	846.8	847.2	848.7	850.9
38	NC+CC, Str	850.7	850.7	848.4	848.4	846.9	848.3	850.7	851.5
39	NC+CC, Str	852.5	852.4	850.6	850	849	850.6	852.4	853.5
40	NC Str; CH2 Tw	858.9	856	853	850.5	850	853.3	856	859.9
41	NC Str; CCN ,Be	859.3	858.2	857	851.6	850.7	857.1	858.2	860.8
42	NC Str; CCN, Be	863.4	863.5	864	861.2	861.4	864.2	863.5	864.7
43	CH2, Ro; NH2, Tw	952.2	950.8	944.1	941.9	941.4	944.1	951	952.2
44	CH2, Ro; NH2, Tw	956.1	952.5	949.6	945.3	944	949.6	952.5	954.9
45	CH2, Ro; NH2, Tw	971.2	962.7	964.5	957.6	956.2	964.8	962.8	970.3

46	NC ,Str ; NCC, Be	1003.3	1002	999.5	998.8	998	999.5	1001.9	1003.6
47	NC, Str ; NCC, Be	1003.9	1002.5	1000.3	999.8	998.3	1000.3	1002.5	1004.8
48	NC, str ; NCC, Be	1004.1	1002.8	1004.6	1000.7	999.7	1005	1002.8	1006
49	NC +CC, Str	1034.4	1033.5	1034.4	1032.6	1034	1034.7	1033.5	1034.6
50	NC +CC, Str	1035.3	1036.8	1035.8	1035.4	1035.9	1036.1	1036.8	1035.4
51	NC +CC, Str	1045.9	1045	1044.9	1044.7	1044.8	1045	1045	1045.8
52	NC +CC, Str	1063.5	1061.4	1053.3	1047.6	1048.5	1053.4	1061.6	1062.8
53	NH2+CH2, Tw	1074.2	1068.1	1068	1052.9	1053.5	1068.2	1068.3	1073
54	NH2+CH2, Tw	1076.4	1069.5	1071.4	1080.8	1079.6	1071.5	1069.6	1075.5
55	NH2+CH2, Wa	1129	1120.7	1117.8	1113.8	1116.9	1117.9	1120.8	1128.7
56	NH2+CH2, Wa	1131.2	1125.9	1124.4	1116.4	1119	1124.7	1125.9	1131.2
57	NH2+CH2, Wa	1148.5	1139.6	1128.3	1126.2	1129.4	1128.5	1139.7	1148.1
58	NH2+CH2, Wa	1153.4	1144.8	1142.5	1129.3	1133.1	1142.9	1144.7	1154.6
59	NH2+CH2, Wa	1156.7	1146.9	1145	1132	1136.5	1145.4	1147	1155.3
60	NH2, Wa; NCH Be	1197.4	1185	1176.3	1159.4	1166.3	1177	1185	1194.7
61	CH2 +NH2 ,Tw	1257.1	1240.1	1230.7	1227	1227.2	1230.7	1240.2	1257
62	CH2 +NH2, Tw	1258.7	1256.9	1240.9	1228.8	1228.4	1240.9	1256.9	1258.6
63	CH2 +NH2, Tw	1265.4	1263.2	1260.5	1246.4	1246.7	1260.6	1263.3	1264.4
64	CH2 +NH2, Tw	1276.1	1274.7	1272.6	1271.5	1271.5	1272.5	1274.7	1275.8
65	CH2 +NH2, Tw	1277.7	1276.1	1275.3	1272.4	1272.6	1275.5	1276.1	1278.1
66	CH2 +NH2, Tw	1284.6	1279.9	1280.7	1276.2	1277.3	1281.1	1279.9	1284.5
67	CH2 +NH2, Tw	1310.5	1293.5	1287.5	1284.4	1284.3	1287.4	1293.6	1310.8
68	CH2 +NH2, Tw	1312	1309.4	1294.7	1285.2	1285.5	1294.8	1309.4	1311.9
69	CH2 +NH2, Tw	1314.4	1312.6	1313.3	1296.2	1296.7	1313.6	1312.6	1314.2
70	CH2 ,Wa; NH2,Tw	1364.5	1365.1	1365.5	1367.4	1367	1365.6	1365.1	1365.3
71	CH2,Wa; NH2, Tw	1366.2	1365.9	1368	1367.8	1367.4	1367.9	1365.9	1365.9
72	CH2,Wa; NH2,Tw	1367.2	1370.1	1370.2	1370.3	1370	1370.2	1370.2	1366.9
73	CH2,Wa; NH2,Tw	1369.9	1371.4	1371	1376.5	1375.5	1371.3	1371.4	1370.3
74	CH2,Wa; NH2, Tw	1371.9	1373.8	1376.9	1377.6	1377.1	1376.8	1373.9	1371.5
75	CH2,Wa; NH2, Tw	1376.7	1382.3	1381.3	1382.2	1381.4	1381.2	1382.4	1376.4
76	CH2, Sc	1468	1469.4	1471.7	1472.7	1473.8	1470.9	1469.6	1468.9
77	CH2, Sc	1468.6	1470.1	1471.9	1474	1475	1473.3	1470	1470.1
78	CH2, Sc	1471.7	1475	1474.5	1475.5	1476.4	1473.9	1475	1470.6
79	CH2, Sc	1472.7	1475.5	1474.8	1478.2	1476.4	1475.7	1475.5	1473.1
80	CH2, Sc	1476.4	1476.9	1477.5	1479	1476.8	1476.1	1476.9	1474.1
81	CH2, Sc	1478.6	1477.4	1479.1	1480	1478.7	1480.5	1477.4	1474.4
82	NH2, Sc	1644.8	1641.2	1636.6	1643.7	1643.7	1636.8	1641.2	1646
83	NH2, Sc	1654.8	1653.4	1648.7	1647.8	1647	1648.7	1653.4	1655.8
84	NH2, Sc	1663	1659.5	1652.6	1650.6	1648.4	1652.7	1659.6	1663.5
85	NH2, Sc	1665	1660.6	1659.4	1659.2	1657.1	1659.2	1660.7	1665.3
86	NH2, Sc	1670.5	1668	1664.5	1660.6	1657.7	1664.6	1668.1	1670.5
87	NH2, Sc	1671.4	1669.5	1669.7	1663	1659	1669.5	1669.5	1674
88	CH2, sym Str	2947.1	2946.2	2945.4	2944.3	2945	2945.4	2946.3	2947.4
89	CH2, sym Str	2948	2947.5	2945.6	2945.2	2945.5	2945.6	2947.5	2947.5
90	CH2, sym Str	2948.1	2947.6	2946.7	2946.4	2945.9	2946.6	2947.5	2947.7
91	CH2, sym Str	2960.9	2957.7	2956.8	2955.2	2956.6	2956.9	2957.8	2961
92	CH2, sym Str	2961.9	2961	2957.4	2956.8	2957.1	2957.5	2960.9	2961.3
93	CH2, sym Str	2962.9	2961.9	2960.3	2958.7	2958.2	2960.2	2961.8	2962.5
94	CH2, antisym Str	3007.4	2997.6	2995.8	2993.2	2995.2	2995.8	2997.7	3007.5
95	CH2, antisym Str	3008.1	3006	2996.1	2994.9	2995.9	2996.3	3005.9	3007.7
96	CH2, antisym Str	3009.3	3006.1	3003.5	2996.8	2996.7	3003.5	3006.1	3008.8
97	CH2, antisym Str	3026.2	3017.5	3016.2	3012.9	3015.6	3016.2	3017.5	3026.2
98	CH2, antisym Str	3027.8	3024.4	3016.3	3015.2	3016.6	3016.5	3024.3	3026.5

99	CH2, antisym Str	3028.5	3025.1	3021.9	3017.7	3017.2	3021.9	3025	3028.3
100	NH2, sym Str	3056.2	3042.1	3042.9	3158	3166.9	3042.1	3042.1	3055.2
101	NH2, sym Str	3059.3	3045.6	3047.2	3160	3168.4	3047.1	3045.6	3060.5
102	NH2, sym Str	3060.5	3080.3	3178.6	3164.1	3171.2	3177	3080.4	3063.7
103	NH2,sym Str	3064.6	3084.9	3180.2	3165.6	3173.4	3181.2	3085	3068.7
104	NH2,sym Str	3116.2	3200.2	3198.6	3185.6	3191	3197.6	3199.6	3116.8
105	NH2,sym Str	3120.7	3202.6	3200.5	3188.5	3193.8	3200.4	3201.8	3123.4
106	NH2, antisym Str	3353.7	3356.4	3366.4	3388.2	3384.2	3366.1	3356.5	3349.8
107	NH2, antisym Str	3355.7	3364.2	3366.5	3388.3	3384.8	3366.7	3364.2	3351.6
108	NH2, antisym Str	3357.6	3364.9	3385.2	3390.8	3387.3	3384.9	3364.9	3357
109	NH2, antisym Str	3364.1	3365.2	3386.7	3391.8	3387.8	3386.4	3365.3	3359.6
110	NH2, antisym Str	3366.2	3387.3	3388.8	3392.1	3388.1	3388.3	3387.2	3361.3
111	NH2, antisym Str	3368.5	3387.8	3390.7	3394.3	3390.4	3390.2	3387.7	3367.7