Eur. J. Inorg. Chem. **2015** · ISSN 1099–0682

SUPPORTING INFORMATION

DOI: 10.1002/ejic.201500756
Title: Towards Cardiolite-Inspired Carbon Monoxide Releasing Molecules – Reactivity of d^4, d^5 Rhenium and d^6 Manganese Carbonyl Complexes with Isocyanide Ligands
Author(s): Emmanuel Kottelat, Valentin Chabert, Aurélien Crochet, Katharina M. Fromm, Fabio Zobi*

Starting complex

Coordinates

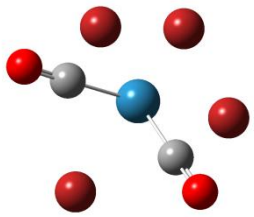
ReIIIAA-3 freq
Created by GaussView 3.09
#

#
#

@<TRIPOS>MOLECULE
Molecule Name
9 4
SMALL
NO_CHARGES

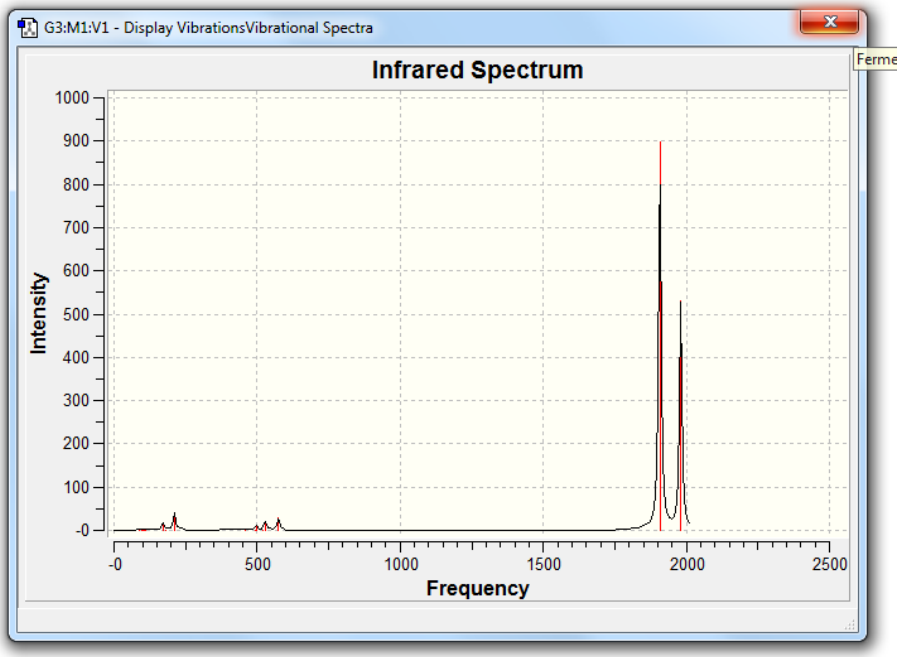
@<TRIPOS>ATOM
1 Re1 -0.0004 -0.0001 -0.1962 Re
2 Br2 -2.5605 0.0038 -0.7956 Br
3 Br3 -0.0031 -1.8132 1.7135 Br
4 Br4 0.0068 1.8163 1.7102 Br
5 Br5 2.5589 -0.0056 -0.7995 Br
6 C6 0.0015 1.5282 -1.3701 C
7 C7 -0.0039 -1.5306 -1.3675 C
8 O8 0.0023 2.4904 -2.0557 O
9 O9 -0.0058 -2.4938 -2.0517 O
@<TRIPOS>BOND
1 1 6 1
2 1 7 1
3 6 8 2
4 7 9 2

Molecular view



IR spectrum

#	Freq	Infrared
1	31.7802	0
2	54.8987	0.1327
3	65.2833	0.0335
4	67.2968	0.5881
5	87.7612	1.2025
6	95.6326	0.3792
7	102.434	2.1126
8	107.35	0.1133
9	108.13	0
10	171.056	17.2846
11	181.871	1.14
12	211.076	29.7997
13	211.247	12.3758
14	460.367	2.3291
15	495.496	1.2145
16	497.915	8.7081
17	518.772	0.001
18	529.008	20.5686
19	574.968	28.4277
20	1907.37	898.261
21	1980.31	531.338



ic1

Coordinates

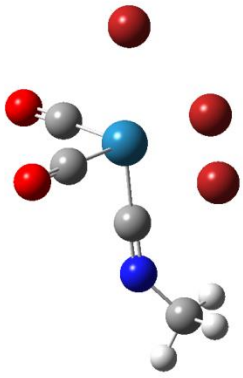
REIAA_L1_CC-4 freq
Created by GaussView 3.09
#

#
#

@<TRIPOS>MOLECULE
Molecule Name
14 10
SMALL
NO_CHARGES

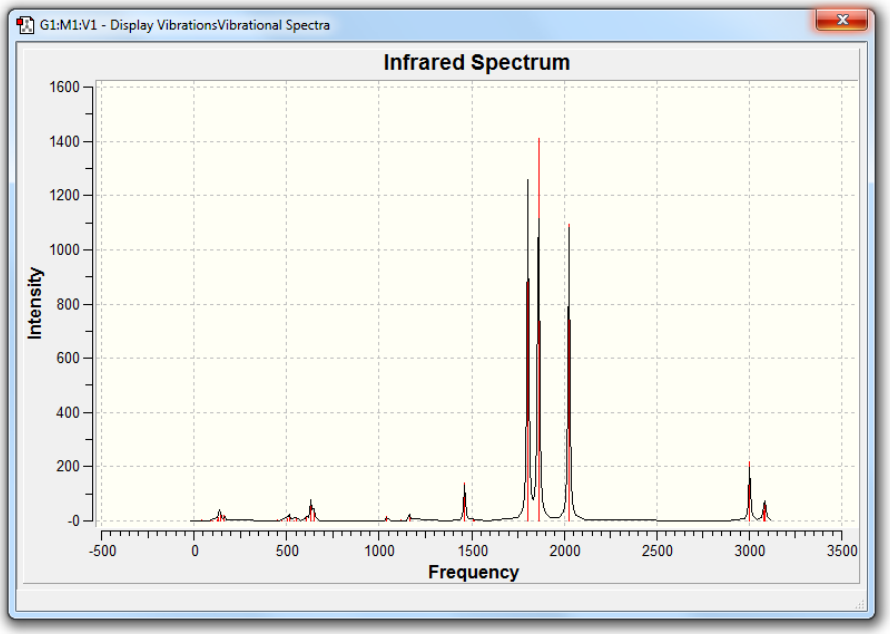
@<TRIPOS>ATOM
1 Re1 0.1098 -0.0001 0.4631 Re
2 C2 0.5828 -1.3606 1.6723 C
3 C3 0.5842 1.3596 1.6727 C
4 C4 -1.7359 0.0005 0.9800 C
5 N5 -2.9196 0.0006 1.2844 N
6 C6 -4.2347 -0.0001 0.6995 C
7 H7 -4.3753 0.8866 0.0630 H
8 H8 -4.3765 -0.8903 0.0680 H
9 H9 -5.0069 0.0026 1.4819 H
10 Br10 2.6770 -0.0009 -0.6169 Br
11 Br11 -0.7527 2.0309 -1.3338 Br
12 Br12 -0.7540 -2.0295 -1.3348 Br
13 O13 0.8627 -2.2214 2.4691 O
14 O14 0.8651 2.2199 2.4698 O
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 2 13 2
5 3 14 2
6 4 5 2
7 5 6 1
8 6 7 1
9 6 8 1
10 6 9 1

Molecular view



IR spectrum

#	Freq	Infrared
1	10.3454	1.0013
2	34.4781	1.1056
3	40.0292	4.8105
4	54.2872	0.8651
5	59.0802	0.4064
6	67.8643	0.3211
7	68.0013	0.1384
8	78.693	0.035
9	87.0858	0.8596
10	102.411	1.7819
11	123.028	3.1481
12	134.451	14.0502
13	134.487	13.8168
14	141.534	29.7344
15	164.373	19.3219
16	448.605	4.3291
17	474.813	4.8446
18	502.909	8.8742
19	515.051	24.3402
20	541.97	0.4014
21	551.269	12.8729
22	606.767	11.3773
23	631.158	75.1359
24	646.743	44.3203
25	1041.62	15.9392
26	1120.52	3.0469
27	1165.68	24.5968
28	1462.3	141.777
29	1511.73	3.6443
30	1517.33	5.9027
31	1803.89	1247.52
32	1861.28	1411.7
33	2025.75	1093.24
34	3002.28	216.974
35	3078.09	37.6365
36	3086.45	66.917



ic2

Coordinates

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# REIIAA_L1_CC-7 freq
# Created by GaussView 3.09
#

#
#

@<TRIPOS>MOLECULE
Molecule Name
14 10
SMALL
NO_CHARGES


@<TRIPOS>ATOM
1 Re1     0.0183    -0.0002     0.3380 Re
2 C2      0.2741    -1.4616     1.5498 C
3 C3      0.2744     1.4614     1.5495 C
4 C4     -1.9076     0.0002     0.7715 C
5 N5     -3.0707     0.0003     1.0270 N
6 C6     -4.4805     0.0023     1.2022 C
7 H7     -4.8109     0.9363     1.6747 H
8 H8     -4.9789    -0.0896     0.2286 H
9 H9     -4.7932    -0.8398     1.8329 H
10 Br10     2.7072     0.0001     0.1302 Br
11 Br11    -0.4487     1.8778    -1.5427 Br
12 Br12    -0.4500    -1.8781    -1.5424 Br
13 O13      0.4024    -2.3799     2.2945 O
14 O14      0.4029     2.3799     2.2939 O
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 2 13 2
5 3 14 2
6 4 5 2
7 5 6 1
8 6 7 1
9 6 8 1
10 6 9 1
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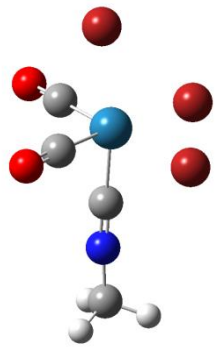
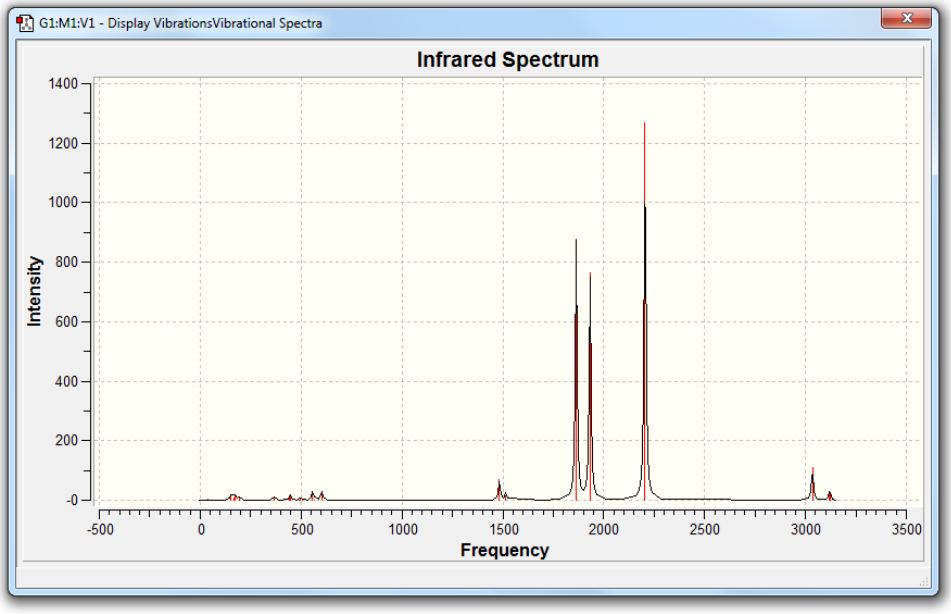
Molecular view



IR spectrum

#	Freq	Infrared
1	23.1205	0.0254
2	38.2167	2.7598
3	40.0283	2.4512
4	45.3886	0.35
5	65.251	0.2681
6	74.0115	0.7843
7	79.6968	0.703
8	83.6747	0.4403
9	91.4595	1.3783
10	99.5386	0.1654
11	151.267	3.2143
12	153.945	18.8771
13	164.925	6.7969
14	173.768	13.903
15	193.378	8.7546
16	365.901	12.3174
17	444.368	9.615
18	447.47	10.5018
19	488.553	1.7758
20	495.437	7.2439
21	506.568	0.3189
22	556.962	30.4598
23	568.486	1.7274
24	602.989	30.2775
25	1041	0.882
26	1158.56	1.102
27	1164.67	0.066
28	1482.97	70.7304
29	1514.22	12.5187
30	1515.89	12.9461
31	1863.79	875.546
32	1932.61	762.619
33	2205.19	1270.12
34	3034.4	110.452
35	3118.3	18.9509
36	3121.66	17.5137



ic3

Coordinates

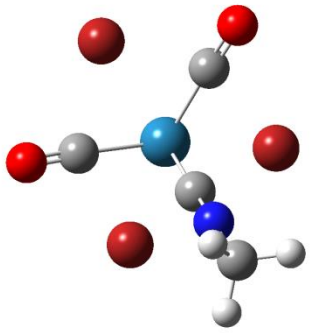
REIIIAA_L1_CC-9 freq
Created by GaussView 3.09
#

#
#

@<TRIPOS>MOLECULE
Molecule Name
14 10
SMALL
NO_CHARGES

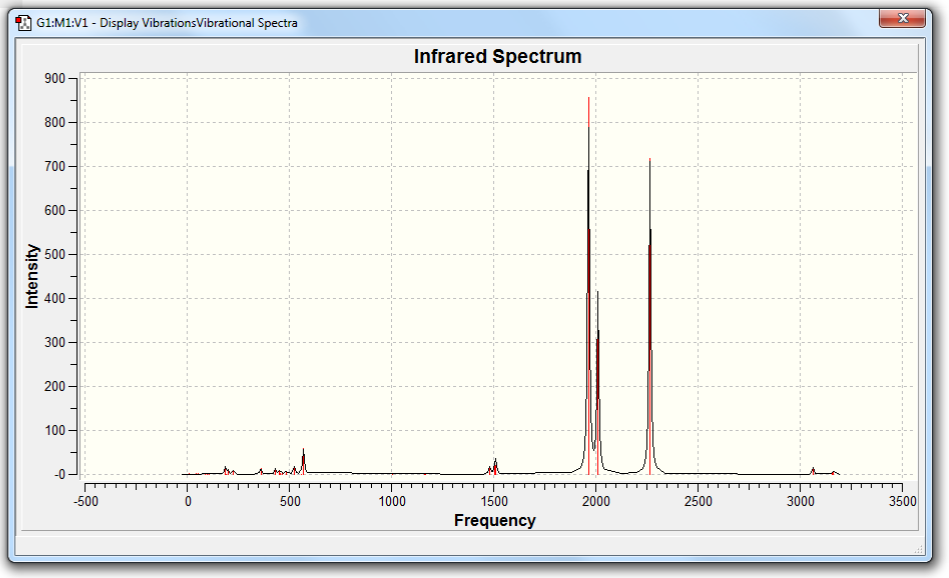
@<TRIPOS>ATOM
1 Re1 0.0253 -0.0092 -0.1984 Re
2 C2 0.2766 1.5293 -1.3801 C
3 C3 0.2367 -1.6310 -1.2713 C
4 C4 -1.7962 -0.0130 -1.0006 C
5 N5 -2.8881 -0.0144 -1.4486 N
6 C6 -4.2286 -0.0071 -1.9493 C
7 H7 -4.8302 -0.7437 -1.4062 H
8 H8 -4.6704 0.9866 -1.8207 H
9 H9 -4.2265 -0.2643 -3.0143 H
10 Br10 2.6343 -0.0512 -0.5174 Br
11 Br11 -0.5103 -1.7075 1.6964 Br
12 Br12 -0.4284 1.8369 1.5777 Br
13 O13 0.3915 2.4764 -2.0640 O
14 O14 0.3288 -2.6258 -1.8876 O
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 4 1
4 2 13 2
5 3 14 2
6 4 5 3
7 5 6 1
8 6 7 1
9 6 8 1
10 6 9 1

Molecular view



IR spectrum

#	Freq	Infrared
1	4.2722	0.2438
2	12.1811	1.9621
3	45.1023	2.8248
4	54.2123	1.5999
5	59.0458	0.8088
6	89.5765	0.8375
7	97.4291	0.299
8	100.117	0.0601
9	105.519	1.0095
10	109.871	0.1063
11	184.626	0.1717
12	188.155	18.3044
13	191.853	0.5703
14	200.512	7.449
15	226.893	8.9755
16	360.487	13.8066
17	432.117	12.7796
18	449.3	6.8504
19	456.78	1.7049
20	463.862	1.6988
21	483.636	7.1522
22	523.64	16.7867
23	557.292	0.3285
24	569.589	59.6524
25	1004.76	0.4614
26	1162.36	0.6137
27	1164.58	0.8369
28	1480.87	17.8669
29	1506.48	20.4761
30	1510.85	21.5734
31	1964.16	857.541
32	2010.37	411.12
33	2265.19	717.985
34	3062.61	16.2279
35	3158.76	3.7076
36	3161.62	3.8438

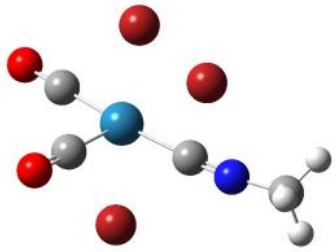


it1

Coordinates

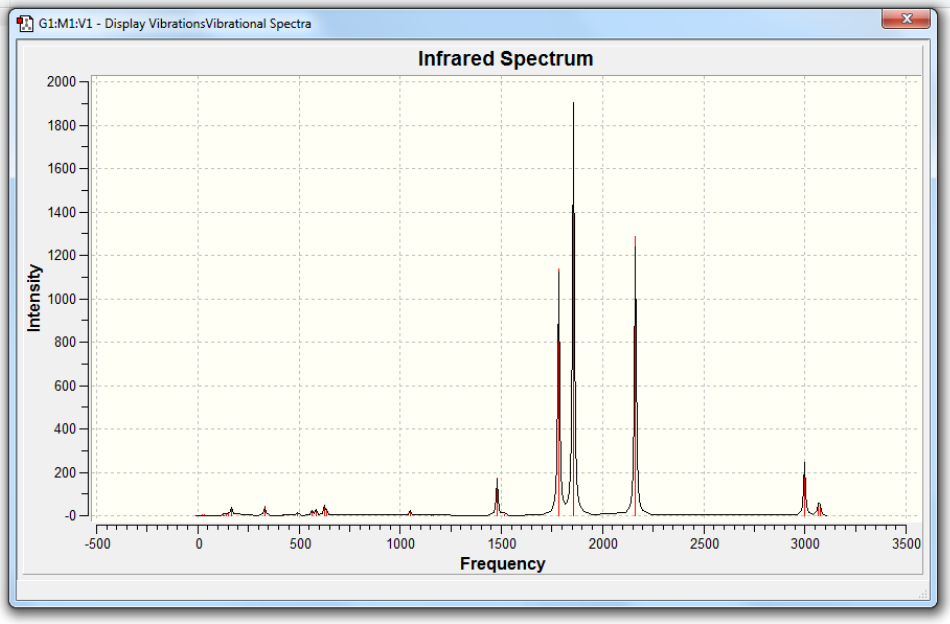
```
# Molecule Name
# Created by GaussView 3.09
#

#
#

@<TRIPOS>MOLECULE
Molecule Name
14 10
SMALL
NO_CHARGES


@<TRIPOS>ATOM
1 Re1    -0.0189    -0.3809    -0.1594 Re
2 Br2     2.7688    -0.3374    -0.1425 Br
3 Br3     0.0138     1.2717     2.1643 Br
4 Br4    -2.7923    -0.1392    -0.2125 Br
5 C5     -0.0884    -1.9651     0.9453 C
6 C6     -0.0362    -1.3895    -1.7203 C
7 O7     -0.1289    -2.9534     1.6272 O
8 O8     -0.0476    -2.0413    -2.7493 O
9 C9      0.0709     1.3880    -1.1344 C
10 N10     0.1347     2.4560    -1.6756 N
11 C11     0.2703     3.7978    -2.0962 C
12 H12     0.8836     4.3687    -1.3828 H
13 H13     0.7528     3.8560    -3.0840 H
14 H14    -0.7120     4.2898    -2.1683 H
@<TRIPOS>BOND
1 1 5 1
2 1 6 1
3 1 9 1
4 5 7 2
5 6 8 2
6 9 10 2
7 10 11 1
8 11 12 1
9 11 13 1
10 11 14 1
```

Molecular view



IR spectrum

#	Freq	Infrared
1	22.4179	3.9508
2	28.1662	0.0958
3	29.9473	3.6007
4	50.1685	0.1938
5	64.8491	0.0117
6	67.1186	0.0957
7	72.6562	0.0362
8	77.1218	0.3595
9	86.1529	0.3353
10	102.902	1.2361
11	125.87	6.8108
12	133.02	0.7286
13	142.18	3.0716
14	152.799	13.6778
15	168.159	38.8927
16	330.277	42.8029
17	420.426	3.8563
18	425.349	3.9175
19	492.56	12.3884
20	563.378	25.4529
21	565.526	0.1059
22	584.765	25.6676
23	626.356	43.4694
24	637.395	19.6704
25	1051.12	24.3675
26	1151.7	1.6686
27	1163.93	2.4378
28	1479.01	171.096
29	1513.14	5.8421
30	1517.6	7.0598
31	1783.52	1134.94
32	1856.39	1901.9
33	2162.49	1287.57
34	2998.3	245.418
35	3066.96	48.976
36	3075.34	40.3197



it2

Coordinates

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#
#

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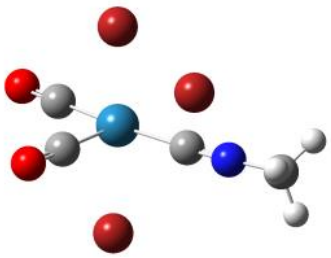
Molecule Name
14 10
SMALL
NO_CHARGES

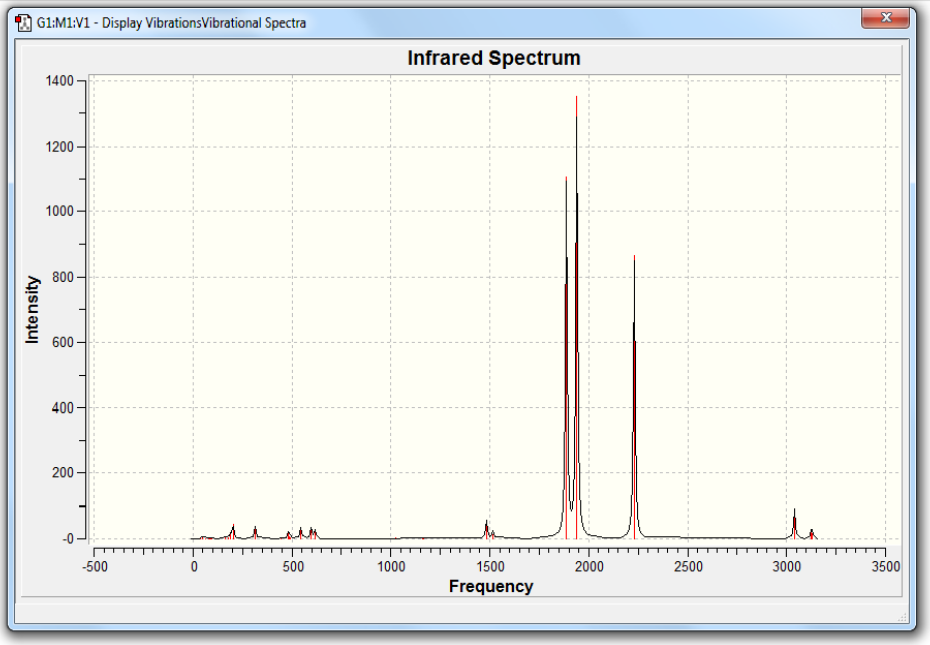

@<TRIPOS>ATOM
1 Re1    -0.0045    -0.2982    -0.1063 Re
2 Br2     2.6607    -0.3049    -0.3668 Br
3 Br3     0.0036     0.9139     2.2907 Br
4 Br4    -2.6673    -0.2486    -0.3793 Br
5 C5     -0.0240    -2.0074     0.8107 C
6 C6     -0.0089    -1.1664    -1.8337 C
7 O7     -0.0355    -3.0465     1.3840 O
8 O8     -0.0114    -1.7087    -2.8906 O
9 C9      0.0192     1.6051    -0.8406 C
10 N10     0.0331     2.7308    -1.2170 N
11 C11     0.0705     4.1087    -1.5623 C
12 H12     0.6314     4.6720    -0.8061 H
13 H13     0.5580     4.2478    -2.5354 H
14 H14    -0.9467     4.5163    -1.6183 H
@<TRIPOS>BOND
1 1 5 1
2 1 6 1
3 1 9 1
4 5 7 2
5 6 8 2
6 9 10 3
7 10 11 1
8 11 12 1
9 11 13 1
10 11 14 1
```

Molecular view



IR spectrum

#	Freq	Infrared
1	18.5073	0.0133
2	40.0747	3.205
3	46.141	3.2287
4	49.7428	0.0605
5	65.1369	0.4552
6	66.3194	0.0683
7	78.9936	0.0109
8	85.8451	0.0305
9	91.1556	0.3188
10	97.3359	0.3291
11	164.805	4.9949
12	177.283	3.9724
13	177.712	1.0112
14	189.845	11.8821
15	202.911	44.0817
16	314.351	38.5134
17	428.797	1.2851
18	442.583	1.5449
19	482.489	16.3406
20	486.141	7.9337
21	491.929	1.997
22	545.145	36.2471
23	597.752	34.2678
24	617.022	27.9027
25	1027.31	3.8941
26	1162.05	0.686
27	1167.9	0.8139
28	1483.85	58.0054
29	1514.91	12.0927
30	1516.93	12.5478
31	1887.19	1106.17
32	1939.84	1351.52
33	2230.39	865.443
34	3040.23	91.5223
35	3125.7	19
36	3127.9	17.3895



it3

Coordinates

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# ReIIIAA_L1_ct-6 freq
# Created by GaussView 3.09
#

#
#

@<TRIPOS>MOLECULE
Molecule Name
14 11
SMALL
NO_CHARGES


@<TRIPOS>ATOM
1 Re1    -0.0011    -0.2243    -0.0391 Re
2 Br2     2.5403    -0.3079    -0.5638 Br
3 Br3     0.0008     0.4941     2.4160 Br
4 Br4    -2.5428    -0.2891    -0.5654 Br
5 C5     -0.0078    -2.0811     0.5659 C
6 C6     -0.0025    -0.7563    -1.9682 C
7 O7     -0.0115    -3.1904     0.9517 O
8 O8     -0.0033    -1.0685    -3.0972 O
9 C9      0.0068     1.7810    -0.4860 C
10 N10     0.0114     2.9397    -0.7070 N
11 C11     0.0211     4.3501    -0.9425 C
12 H12     0.6334     4.8487    -0.1836 H
13 H13     0.4381     4.5606    -1.9331 H
14 H14    -1.0000     4.7431    -0.8939 H
@<TRIPOS>BOND
1 1 3 1
2 1 5 1
3 1 6 1
4 1 9 1
5 5 7 2
6 6 8 2
7 9 10 3
8 10 11 1
9 11 12 1
10 11 13 1
11 11 14 1
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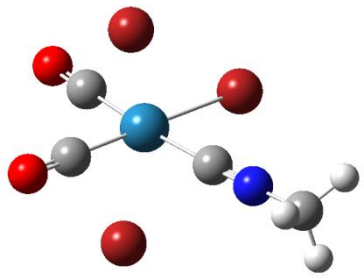
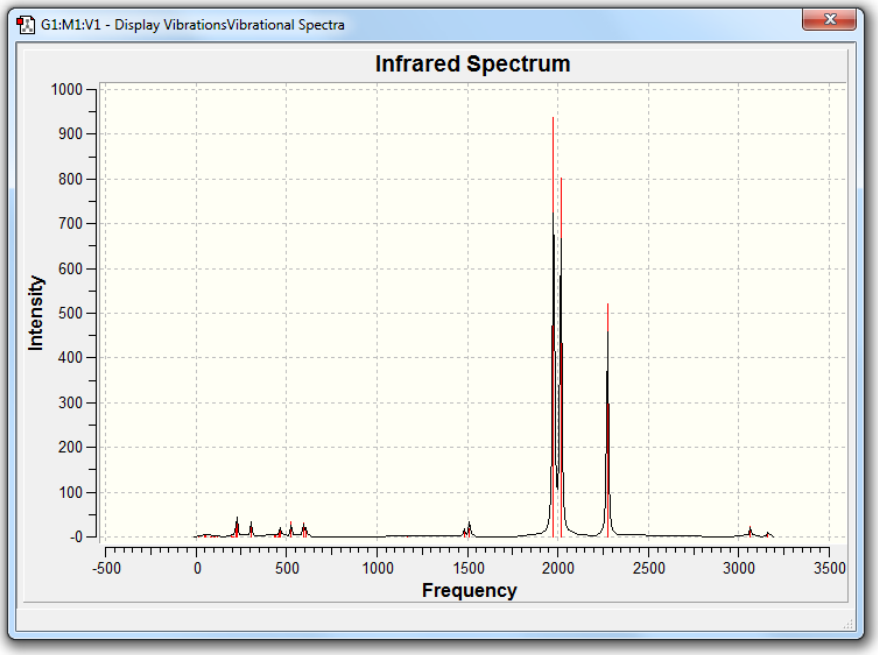
Molecular view



IR spectrum

#	/	Freq	Infrared
1		18.432	0.0027
2		46.79	4.3212
3		49.1253	0.0602
4		51.9826	3.2916
5		54.0355	0.569
6		82.4908	0.1099
7		87.0502	0.094
8		97.2049	0.0969
9		105.412	0.0395
10		116.164	0.8987
11		192.635	1.41
12		201.364	0.3492
13		206.807	0.6529
14		223.625	18.4801
15		227.748	33.4211
16		304.764	33.0076
17		436.199	2.795
18		437.34	1.6839
19		450.221	0.258
20		460.449	9.392
21		466.545	16.6813
22		526.544	32.6858
23		592.861	30.6051
24		607.652	16.5587
25		996.349	0.016
26		1165.58	0.4031
27		1167.67	0.4165
28		1483.75	16.7304
29		1511.39	18.7875
30		1512.03	18.8178
31		1976.23	936.41
32		2016.12	802.638
33		2274.31	521.029
34		3063.9	23.0052
35		3159.39	5.4339
36		3160.43	4.9834



icc1

Coordinates

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# Created by GaussView 3.09
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#
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@<TRIPOS>MOLECULE
Molecule Name
19 16
SMALL
NO_CHARGES


@<TRIPOS>ATOM
1 Re1     0.1104    -0.3678     0.2513 Re
2 Br2    -2.5674    -0.4762    -0.4428 Br
3 Br3     0.6740     1.1602    -2.0240 Br
4 C4     -0.2097    -1.3282     1.8463 C
5 C5      0.4189    -1.9993    -0.7767 C
6 O6     -0.3901    -1.9286     2.8715 O
7 O7      0.5908    -2.9882    -1.4123 O
8 C8     -0.4354     1.4301     1.0547 C
9 C9      2.0060    -0.1307     0.6343 C
10 N10    -0.8110     2.4845     1.4581 N
11 N11     3.1750     0.0283     0.8664 N
12 C12    -1.4028     3.7434     1.7492 C
13 H13    -2.3752     3.6034     2.2384 H
14 H14    -0.7576     4.3320     2.4141 H
15 H15    -1.5595     4.3084     0.8215 H
16 C16     4.5686     0.2934     0.7887 C
17 H17     5.0271     0.2753     1.7871 H
18 H18     5.0764    -0.4582     0.1668 H
19 H19     4.7534     1.2813     0.3425 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 8 1
4 1 9 1
5 4 6 2
6 5 7 2
7 8 10 3
8 9 11 2
9 10 12 1
10 11 16 1
11 12 13 1
12 12 14 1
13 12 15 1
14 16 17 1
15 16 18 1
16 16 19 1
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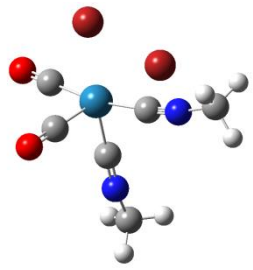
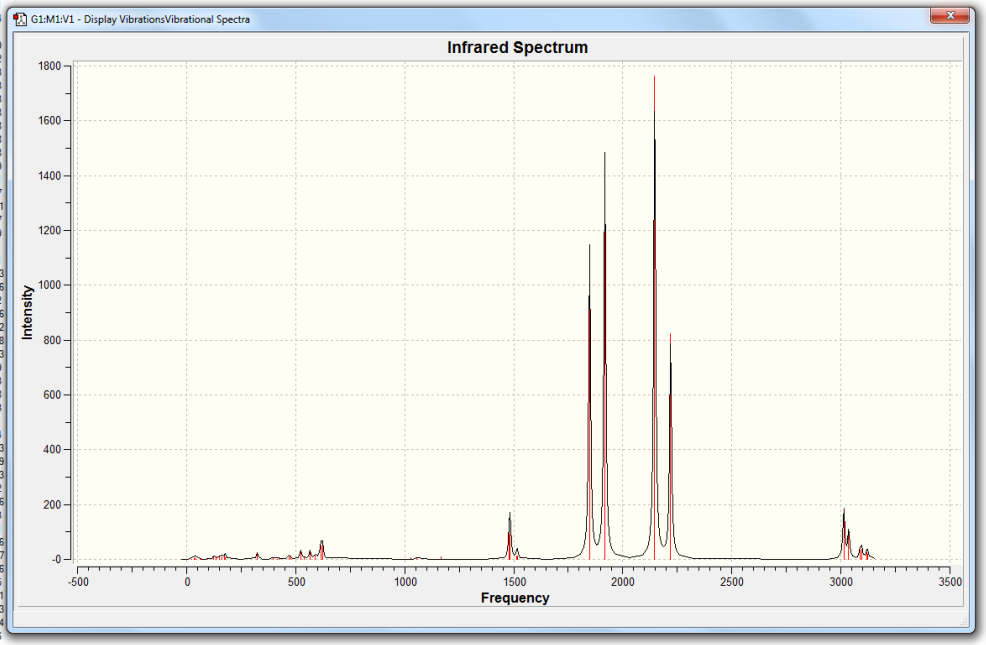
Molecular view



IR spectrum

#	Freq	Infrared
1	9.1859	0.08
2	23.8292	0.2434
3	34.1213	3.4141
4	38.8723	5.2274
5	40.2383	4.888
6	46.6258	1.4979
7	63.8443	0.5722
8	67.5309	0.0693
9	74.5089	0.2013
10	83.1671	0.1463
11	97.5305	0.4058
12	123.541	9.1318
13	133.587	8.3458
14	150.306	8.6388
15	162.286	9.8609
16	175.571	14.341
17	179.213	6.8327
18	324.111	25.8381
19	395.131	6.8067
20	414.739	1.4829
21	423.792	1.825
22	469.017	9.4641
23	475.97	11.8313
24	522.765	33.5506
25	539.203	6.9562
26	565.471	31.3606
27	590.79	15.4972
28	615.394	49.4268
29	623.354	55.7863
30	1029.09	4.6619
31	1054.35	4.5953
32	1148.02	0.8388
33	1156.35	1.1413
34	1166.43	8.024
35	1168.41	2.2674
36	1480.68	102.723
37	1484.18	89.0159
38	1513.97	11.1033
39	1516.42	8.5112
40	1516.64	12.4576
41	1516.72	8.3483
42	1848.07	1146.1
43	1917.88	1480.76
44	2146.26	1762.37
45	2219.2	824.916
46	3013.55	186.25
47	3035.71	107.211
48	3089.07	33.4913
49	3095.34	36.1344
50	3118.89	25.126
51	3123.59	18.2311



icc2

Coordinates

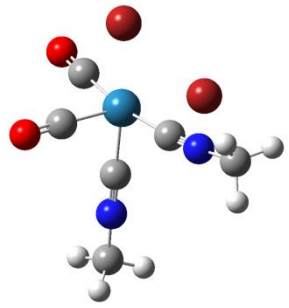
```
# Title Card Required
# Created by GaussView 3.09
#

#
#

@<TRIPOS>MOLECULE
Molecule Name
19 16
SMALL
NO_CHARGES

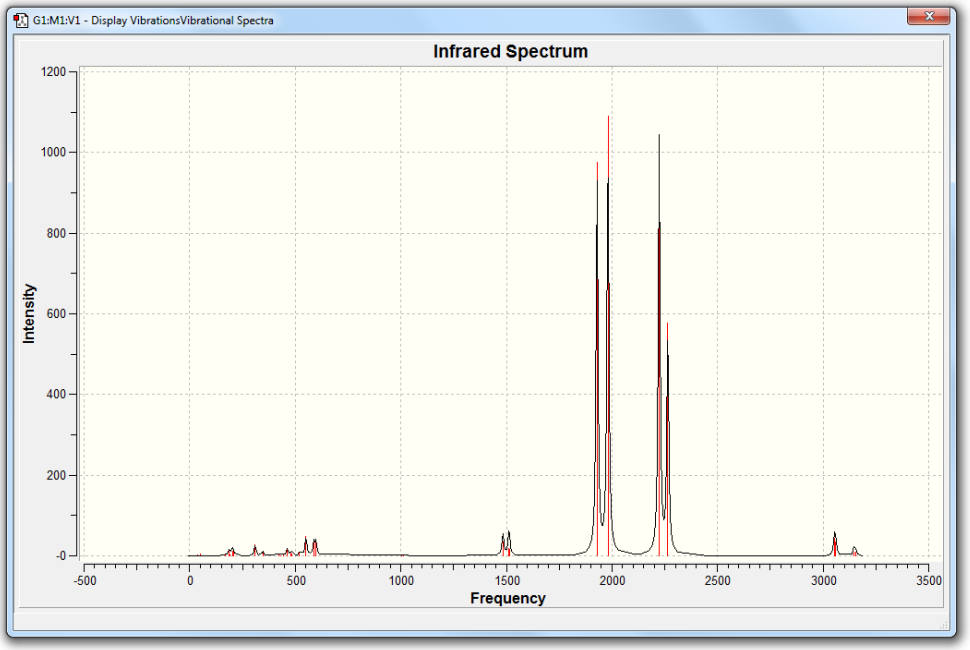

@<TRIPOS>ATOM
1 Re1    -0.0553   -0.2715   -0.2013 Re
2 Br2     2.5665   -0.5256    0.1309 Br
3 Br3    -0.7303    0.6490    2.2002 Br
4 C4      0.2602   -0.8840   -2.0185 C
5 C5     -0.2963   -2.0928    0.4904 C
6 O6      0.4215   -1.2486   -3.1311 O
7 O7     -0.4276   -3.1769    0.9297 O
8 C8      0.3552    1.6950   -0.6513 C
9 C9     -2.0008   -0.0874   -0.6425 C
10 N10    0.6399    2.8251   -0.8471 N
11 N11   -3.1528    0.0115   -0.9049 N
12 C12    1.0461    4.1850   -1.0101 C
13 H13    2.0138    4.2271   -1.5219 H
14 H14    0.3054    4.7338   -1.6020 H
15 H15    1.1427    4.6626   -0.0289 H
16 C16   -4.5571    0.1101   -1.1438 C
17 H17   -4.7448    0.5872   -2.1124 H
18 H18   -5.0138   -0.8862   -1.1442 H
19 H19   -5.0256    0.7125   -0.3569 H
@<TRIPOS>BOND
1 1 4 1
2 1 5 1
3 1 8 1
4 1 9 1
5 4 6 2
6 5 7 2
7 8 10 3
8 9 11 3
9 10 12 1
10 11 16 1
11 12 13 1
12 12 14 1
13 12 15 1
14 16 17 1
15 16 18 1
16 16 19 1
```

Molecular view



IR spectrum

#	/	Freq	Infrared
1		26.022	0.0161
2		26.3799	0.0275
3		37.7904	3.35
4		45.0302	0.4971
5		49.0288	2.5006
6		51.7525	4.9456
7		68.5166	0.2308
8		75.9335	0.1983
9		82.7779	0.2735
10		86.8723	0.1469
11		91.5296	0.2024
12		167.125	2.17
13		186.375	11.6911
14		190.279	2.8683
15		192.893	1.9779
16		203.393	11.2496
17		206.649	9.1022
18		310.054	27.1136
19		348.161	11.2515
20		420.481	1.3324
21		431.119	0.2873
22		442.808	4.0677
23		461.476	16.214
24		480.663	6.0794
25		484.269	5.2267
26		520.717	9.3688
27		551.055	47.1021
28		588.318	32.1137
29		598.12	34.323
30		1001.69	0.1308
31		1012.16	0.8646
32		1160.83	0.1686
33		1162.98	0.5356
34		1164.79	0.5925
35		1168.26	0.4634
36		1482.66	33.7984
37		1484.9	23.4138
38		1511.18	18.467
39		1512.25	17.0045
40		1513.58	17.0335
41		1514.14	17.1609
42		1929.35	976.22
43		1980.98	1089.17
44		2223.63	1037.34
45		2264.54	578.051
46		3053.72	44.2178
47		3059.58	34.135
48		3146.13	9.4756
49		3147	8.4318
50		3152.9	8.6857
51		3154.54	6.1221



icc3

Coordinates

```
# ReIII (CO)2 Br2 (isopropL)2 ccc
# Created by GaussView 3.09
#

#
#

@<TRIPOS>MOLECULE
Molecule Name
19 17
SMALL
NO_CHARGES


@<TRIPOS>ATOM
1 Re1     0.0087   -0.1978    0.0615 Re
2 Br2    -2.4079   -1.0317   -0.1546 Br
3 Br3     0.9953    0.9301   -1.9945 Br
4 C4     -0.3469   -0.6695    1.9592 C
5 C5      0.5349   -1.9734   -0.6695 C
6 O6     -0.5351   -0.8935    3.0890 O
7 O7      0.8343   -2.9991   -1.1349 O
8 C8     -0.6770    1.7002    0.5385 C
9 C9      1.8927   -0.1212    0.8287 C
10 N10   -1.1080    2.7728    0.7520 N
11 N11    2.9878   -0.0957    1.2555 N
12 C12   -1.6530    4.0832    0.9775 C
13 H13   -2.7289    4.0052    1.1632 H
14 H14   -1.1683    4.5401    1.8461 H
15 H15   -1.4811    4.7073    0.0951 H
16 C16    4.3416   -0.0663    1.7396 C
17 H17    4.3898    0.5018    2.6735 H
18 H18    4.6918   -1.0890    1.9123 H
19 H19    4.9814    0.4106    0.9896 H
@<TRIPOS>BOND
1 1 3 1
2 1 4 1
3 1 5 1
4 1 8 1
5 1 9 1
6 4 6 2
7 5 7 2
8 8 10 3
9 9 11 3
10 10 12 1
11 11 16 1
12 12 13 1
13 12 14 1
14 12 15 1
15 16 17 1
16 16 18 1
17 16 19 1
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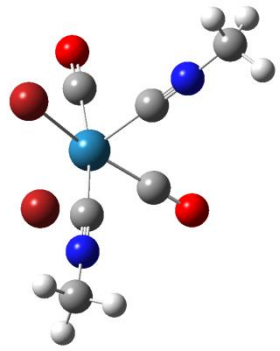
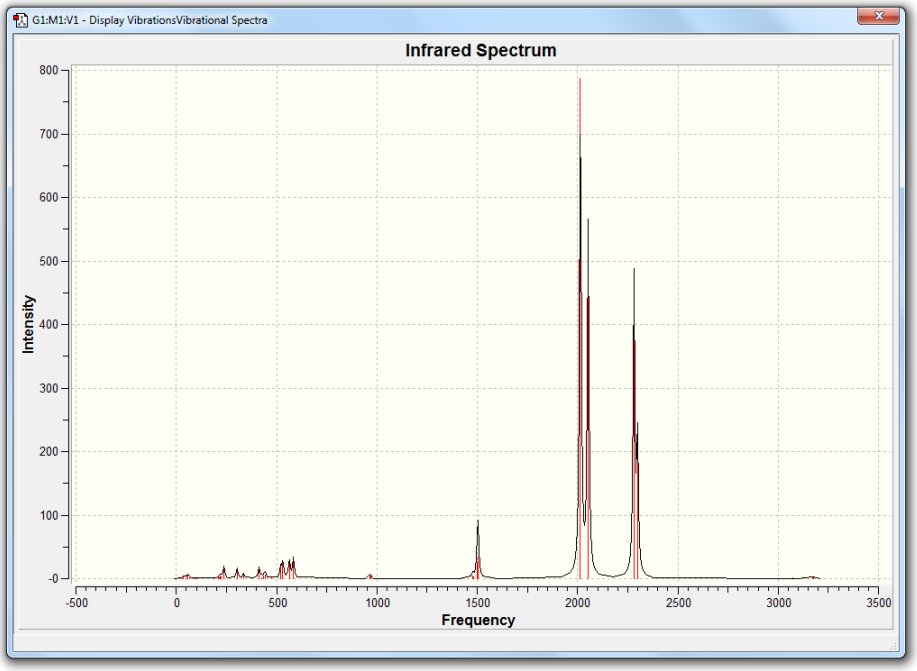
Molecular view



IR spectrum

#	Freq	Infrared
1	18.912	0.0022
2	29.1171	0.1005
3	36.4164	4.5338
4	49.8527	2.095
5	55.2634	0.1642
6	58.0484	5.0609
7	64.1161	1.7231
8	86.7402	0.1736
9	89.8312	0.2066
10	99.3564	0.1608
11	104.292	0.4337
12	187.343	1.6293
13	207.993	2.6138
14	215.626	0.905
15	219.711	3.5733
16	223.346	2.6175
17	237.904	18.859
18	302.996	16.8759
19	334.798	8.9014
20	412.715	17.9821
21	425.524	1.1656
22	435.503	4.6346
23	443.556	5.983
24	445.008	3.485
25	477.426	0.8369
26	520.898	17.6062
27	531.087	26.3339
28	563.842	29.3285
29	583.955	32.2318
30	964.244	4.2772
31	967.683	3.7236
32	1160.83	0.343
33	1162.61	0.3156
34	1163.12	0.5817
35	1164.95	0.4536
36	1477.04	4.4683
37	1479.91	3.1089
38	1500.94	25.8674
39	1503.36	15.5612
40	1503.88	34.3425
41	1504.85	26.8618
42	2014.24	787.084
43	2052.91	553.375
44	2281.37	478.403
45	2298.86	224.552
46	3070.73	0.1101
47	3072.47	1.0675
48	3170.83	0.7861
49	3173.51	0.6739
50	3175.36	0.4369
51	3176.74	1.424

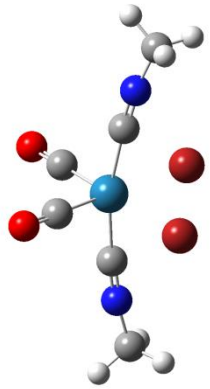


ict1

Coordinates

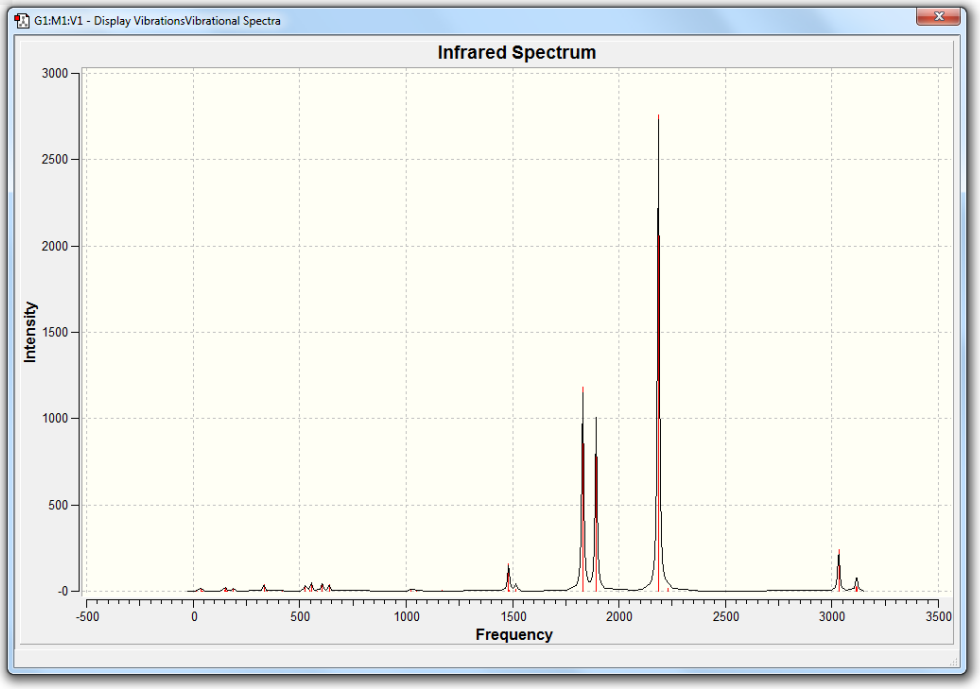
```
# Title Card Required
# Created by GaussView 3.09
#

#
#

@<TRIPOS>MOLECULE
Molecule Name
19 16
SMALL
NO_CHARGES


@<TRIPOS>ATOM
1 Re1     0.0003     0.0010     0.5247 Re
2 C2      0.0036     1.3655     1.8364 C
3 C3     -0.0019    -1.3612     1.8389 C
4 O4     -0.0031    -2.2162     2.6819 O
5 O5      0.0056     2.2220     2.6779 O
6 Br6    -0.0047    -1.9707    -1.4419 Br
7 C7      2.0086    -0.0044     0.2879 C
8 C8     -2.0083     0.0041     0.2897 C
9 N9      3.1792    -0.0068     0.0690 N
10 N10   -3.1791     0.0042     0.0717 N
11 C11    4.5242    -0.0088    -0.3864 C
12 H12    4.6166     0.5960    -1.2980 H
13 H13    5.1936     0.4074     0.3778 H
14 H14    4.8499    -1.0320    -0.6155 H
15 C15   -4.5239     0.0005    -0.3845 C
16 H16   -5.1888    -0.4383     0.3709 H
17 H17   -4.8610     1.0242    -0.5934 H
18 H18   -4.6091    -0.5873    -1.3078 H
19 Br19   0.0031     1.9694    -1.4450 Br
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 7 1
4 1 8 1
5 2 5 2
6 3 4 2
7 7 9 2
8 8 10 2
9 9 11 1
10 10 15 1
11 11 12 1
12 11 13 1
13 11 14 1
14 15 16 1
15 15 17 1
16 15 18 1
```

Molecular view



IR spectrum

#	Freq	Infrared
1	3.5445	0.0876
2	13.9318	0.1221
3	37.2423	9.5802
4	38.8379	9.2385
5	43.2949	0.0088
6	47.1018	1.4698
7	70.7013	0.0742
8	72.1887	0.0422
9	76.3931	0
10	96.0282	2.2172
11	101.877	0.1312
12	147.708	6.8146
13	151.297	16.9994
14	157.726	0.0009
15	162.805	3.0841
16	187.665	10.0172
17	188.828	7.5956
18	332.487	38.3506
19	349.663	3.8165
20	420.192	0.2405
21	420.223	6.8957
22	496.987	0.2292
23	525.86	8.5035
24	527.359	26.8622
25	549.904	4.2863
26	555.879	44.6938
27	583.331	0.0002
28	607.26	45.9708
29	639.099	36.2411
30	1023.22	9.5442
31	1049.68	0.0034
32	1156.86	0.9374
33	1157.29	2.0048
34	1167.72	3.162
35	1167.84	1.0029
36	1481.43	156.229
37	1484.32	4.6827
38	1514.4	10.5269
39	1514.45	9.8117
40	1517.43	11.0302
41	1517.45	12.1269
42	1829.87	1180.32
43	1892.75	1003.38
44	2185.39	2759.62
45	2230.9	17.279
46	3031.73	240.283
47	3032.5	8.6526
48	3114.8	27.6925
49	3114.93	24.9339
50	3117.32	20.9257
51	3117.52	20.973



ict2

Coordinates

```
# Re(CO)2Br2(isopropL)2cct
# Created by GaussView 3.09
#

#
#

@<TRIPOS>MOLECULE
Molecule Name
19 16
SMALL
NO_CHARGES


@<TRIPOS>ATOM
1 Re1     0.0000     0.0001     0.4039 Re
2 C2      0.1462    -1.3417     1.7886 C
3 C3     -0.1460     1.3419     1.7885 C
4 O4     -0.2675     2.1452     2.6484 O
5 O5      0.2678    -2.1449     2.6484 O
6 Br6     0.0814     2.0310    -1.3160 Br
7 C7     -2.0355    -0.0025     0.2076 C
8 C8      2.0355     0.0025     0.2073 C
9 N9     -3.2040     0.0017     0.0315 N
10 N10     3.2040    -0.0020     0.0311 N
11 C11    -4.6042     0.0001    -0.2497 C
12 H12    -4.8490    -0.8333    -0.9175 H
13 H13    -5.1758    -0.1072     0.6788 H
14 H14    -4.8882     0.9400    -0.7357 H
15 C15     4.6043    -0.0007    -0.2498 C
16 H16     5.1756     0.1098     0.6785 H
17 H17     4.8888    -0.9420    -0.7328 H
18 H18     4.8489     0.8307    -0.9201 H
19 Br19   -0.0816    -2.0310    -1.3158 Br
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 7 1
4 1 8 1
5 2 5 2
6 3 4 2
7 7 9 3
8 8 10 3
9 9 11 1
10 10 15 1
11 11 12 1
12 11 13 1
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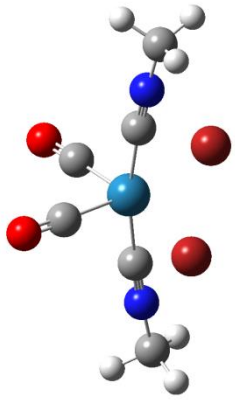
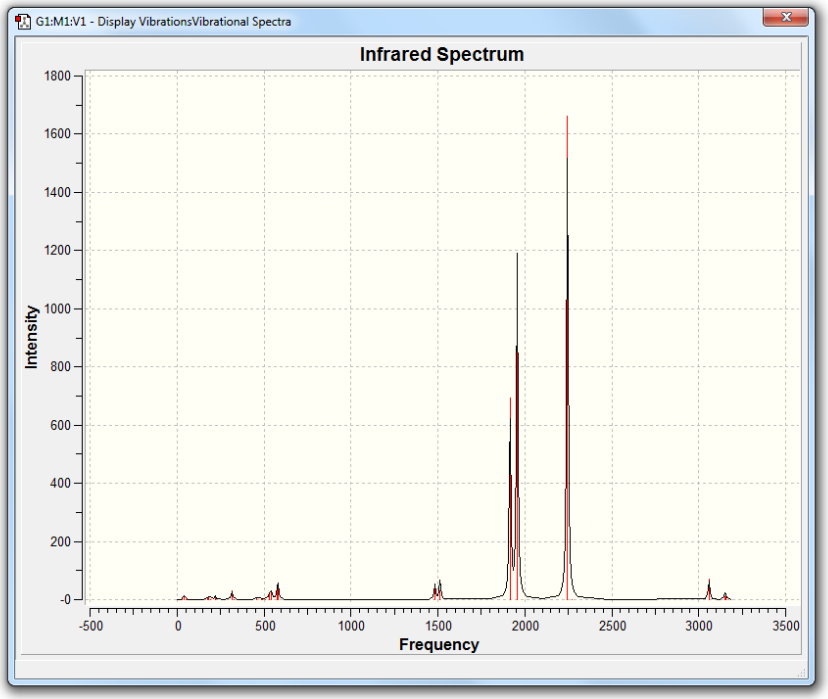
Molecular view



IR spectrum

#	Freq	Infrared
1	29.7751	0.0002
2	29.8415	0.0003
3	41.5991	7.838
4	43.5589	8.7341
5	53.7524	0.0354
6	58.0628	0.9687
7	62.3289	0.1524
8	68.8074	0.1131
9	72.7268	0.0996
10	98.6312	1.6422
11	102.484	0.04
12	177.754	2.875
13	183.903	10.2542
14	183.976	0.0134
15	190.298	0.8365
16	218.676	9.9583
17	219.172	5.806
18	315.168	31.5377
19	330.286	1.4217
20	428.796	0.3341
21	434.038	0.0216
22	456.212	6.5144
23	483.242	2.5688
24	492.83	4.647
25	506.444	0.1113
26	533.251	23.9263
27	543.744	26.5266
28	578.164	31.7096
29	581.85	35.836
30	994.19	0.1671
31	1016.52	0.1701
32	1163.64	0.03
33	1164.12	0.9488
34	1167.63	0.3111
35	1167.91	0.5102
36	1483.25	50.5101
37	1484.61	0.0625
38	1512.15	20.5687
39	1512.16	15.4443
40	1513.41	3.7282
41	1513.44	31.1284
42	1914.97	691.914
43	1956.17	1182.25
44	2245.2	1661.36
45	2271.73	0.2799
46	3058.92	71.255
47	3059.1	0.55
48	3152.68	9.7901
49	3152.69	6.4397
50	3153.64	8.7472
51	3153.66	4.2913



ict3

Coordinates

```
# ReIII(CO)2Br2(isopropL)2 cct IR
# Created by GaussView 3.09
#

#
#

@<TRIPOS>MOLECULE
Molecule Name
19 16
SMALL
NO_CHARGES


@<TRIPOS>ATOM
1 Re1    -0.0000    0.0000    0.2513 Re
2 C2    -0.3938    1.2188    1.7358 C
3 C3    0.3936    -1.2186    1.7359 C
4 O4    0.6768    -1.9219    2.6252 O
5 O5    -0.6771    1.9221    2.6250 O
6 Br6    -0.2658    -2.2093    -1.0299 Br
7 C7    2.0614    -0.0484    0.0297 C
8 C8    -2.0615    0.0484    0.0296 C
9 N9    3.2207    -0.0818    -0.1554 N
10 N10    -3.2207    0.0817    -0.1556 N
11 C11    4.6350    -0.1109    -0.4094 C
12 H12    4.9104    0.7395    -1.0408 H
13 H13    5.1795    -0.0538    0.5384 H
14 H14    4.8945    -1.0435    -0.9207 H
15 C15    -4.6350    0.1105    -0.4096 C
16 H16    -5.1796    0.0091    0.5344 H
17 H17    -4.9016    1.0617    -0.8813 H
18 H18    -4.9034    -0.7147    -1.0764 H
19 Br19    0.2659    2.2093    -1.0300 Br
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 7 1
4 1 8 1
5 2 5 2
6 3 4 2
7 7 9 3
8 8 10 3
9 9 11 1
10 10 15 1
11 11 12 1
12 11 13 1
13 11 14 1
14 15 16 1
15 15 17 1
16 15 18 1
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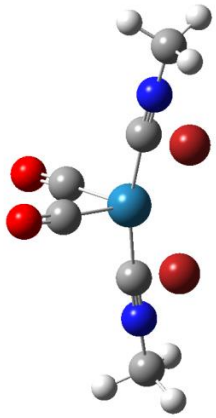
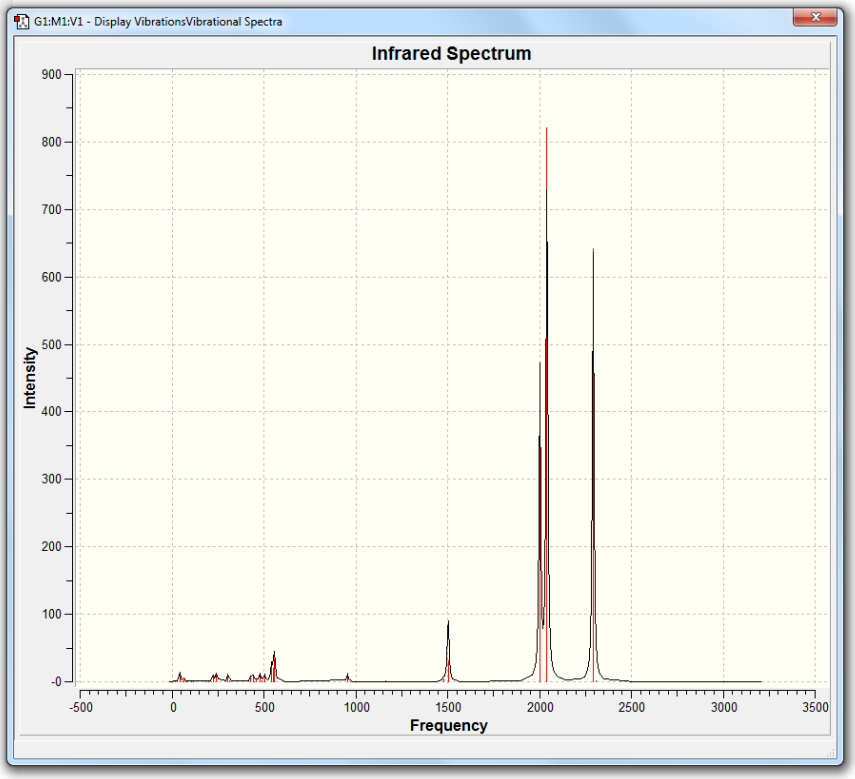
Molecular view



IR spectrum

#	Freq	Infrared
1	18.6195	0.0061
2	28.3101	0.0111
3	41.6316	6.4893
4	42.801	8.5469
5	58.3831	0.6109
6	65.0734	3.3625
7	66.3385	1.4455
8	78.7503	0.0345
9	85.4894	0.5168
10	106.934	0.8196
11	118.522	0.0238
12	183.949	1.1811
13	201.889	0.0435
14	215.835	0.5902
15	224.845	8.0345
16	240.41	3.2182
17	243.191	11.2254
18	305.415	11.2323
19	314.412	1.2757
20	427.601	7.4687
21	441.595	8.814
22	447.33	0.6696
23	459.019	3.0081
24	477.375	12.3311
25	487.2	0.7757
26	504.159	10.7249
27	542.019	23.9931
28	553.268	19.818
29	558.694	33.6581
30	954.638	12.7823
31	973.45	0.1225
32	1163.3	0.0402
33	1163.52	0.7117
34	1164.6	0.1075
35	1164.84	0.8368
36	1478.5	4.5974
37	1479.22	0.016
38	1502.73	28.4996
39	1502.76	20.4251
40	1503.52	25.517
41	1503.58	31.2401
42	2002.14	462.559
43	2040.73	821.42
44	2292.22	642.457
45	2307.11	1.7233
46	3072.71	0.3299
47	3072.76	0.4727
48	3174.11	0.4546
49	3174.15	0.4331
50	3176.73	0.3641
51	3176.81	0.3745



Final product

Coordinates

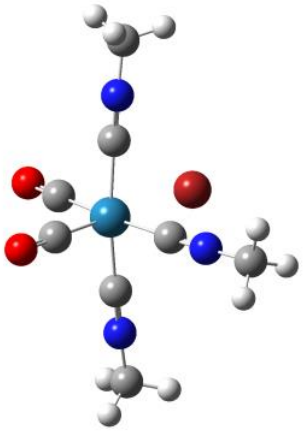
complex 4 ir
Created by GaussView 3.09
#

#
#

@<TRIPOS>MOLECULE
Molecule Name
24 22
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 Re1 0.0007 -0.2916 -0.3656 Re
2 C2 0.0006 -0.6537 -2.2357 C
3 C3 0.0038 -2.1989 0.0985 C
4 O4 0.0056 -3.3450 0.3894 O
5 O5 0.0004 -0.8714 -3.4101 O
6 Br6 0.0006 0.3373 2.3162 Br
7 C7 -2.0330 -0.2559 -0.2152 C
8 C8 -0.0031 1.7502 -0.6439 C
9 C9 2.0346 -0.2498 -0.2163 C
10 N10 -3.2109 -0.2390 -0.0736 N
11 N11 -0.0059 2.9295 -0.7641 N
12 N12 3.2124 -0.2300 -0.0744 N
13 C13 -4.6135 -0.2356 0.1852 C
14 H14 -4.8702 0.5867 0.8633 H
15 H15 -5.1741 -0.1129 -0.7489 H
16 H16 -4.9129 -1.1804 0.6536 H
17 C17 -0.0137 4.3545 -0.8333 C
18 H18 0.9959 4.7299 -1.0365 H
19 H19 -0.6816 4.6926 -1.6341 H
20 H20 -0.3598 4.7740 0.1183 H
21 C21 4.6154 -0.2203 0.1821 C
22 H22 4.9640 -1.2334 0.4144 H
23 H23 5.1616 0.1464 -0.6949 H
24 H24 4.8376 0.4302 1.0360 H
@<TRIPOS>BOND
1 1 2 1
2 1 3 1
3 1 7 1
4 1 8 1
5 1 9 1
6 2 5 2
7 3 4 2
8 7 10 3
9 8 11 3
10 9 12 3
11 10 13 1
12 11 17 1
13 12 21 1
14 13 14 1
15 13 15 1
16 13 16 1
17 17 18 1
18 17 19 1
19 17 20 1
20 21 22 1
21 21 23 1
22 21 24 1

Molecular view



IR spectrum

#	/	Freq	Infrared
1		16.3934	0.0188
2		19.8808	0.04
3		26.2978	0.0083
4		36.104	2.7681
5		43.9994	8.3005
6		45.3577	3.3128
7		48.2149	8.9483
8		49.8977	0.1179
9		69.9332	0.0179
10		70.4282	0.733
11		88.0495	0.7051
12		96.5516	0.4796
13		155.254	1.0325
14		171.082	5.0372
15		171.634	2.6972
16		185.595	1.7576
17		198.961	2.7882
18		200.893	6.5246
19		207.785	9.6841
20		310.729	32.2806
21		320.34	50.3254
22		336.291	1.7858
23		396.839	0.0303
24		424.308	1.1525
25		427.198	0.8837
26		467.126	14.2573
27		498.121	4.8475
28		512.85	5.8014
29		527.625	0.1095
30		543.7	24.118
31		574.721	0.1483
32		576.108	71.8795
33		613.425	67.1965
34		614.808	49.4909
35		1001.14	2.5136
36		1007.37	0.9504
37		1025.77	0.2948
38		1161.98	0.0747
39		1162.78	0.5014
40		1163.06	1.1793
41		1166.62	0.7614
42		1167.06	0.4517
43		1167.14	0.6008
44		1484.28	27.8477
45		1484.55	86.9348
46		1487.95	11.3633
47		1513.74	18.242
48		1514.02	2.6885
49		1514.21	28.0029
50		1515.01	12.8566
51		1515.52	22.1029
52		1515.64	10.8647
53		1882.92	1087.41
54		1949.91	1266.09
55		2212.97	2314.34
56		2221.15	645.42
57		2265.69	187.9
58		3050.54	115.529
59		3050.92	9.0985
60		3052.74	51.6817
61		3140.71	13.48
62		3141.13	12.12
63		3141.65	13.8445
64		3141.74	8.3986
65		3142.96	12.2012
66		3145.04	10.1599