Molecular Structure of Magnesium Dibromide: An Electron Diffraction and Quantum Chemical Study

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Supporting Information

Molecular intensities for two camera ranges of magnesium dibromide

Camera range = 19 cm

$s_{\min} = 9.00 \text{ \AA}^{-1}$ $s_{\max} = 30.00 \text{ \AA}^{-1}$ step size = $0.25 \text{ \AA}^{-1}$

				147.4	23.9	-75.3	-103.9
-112.1	-121.6	-98.5	-30.1	47.5	160.7	149.2	103.3
21.9	-42.7	-64.6	-85.7	-93.4	-81.0	-33.3	34.2
97.0	84.7	59.8	18.3	-15.0	-48.7	-60.9	-54.1
-52.1	-11.0	5.0	43.7	58.1	57.7	25.3	-6.7
-36.3	-46.4	-57.2	-52.4	1.7	31.7	44.6	43.1
40.1	13.7	-8.7	-1.1	-48.5	-26.3	-12.4	-17.1
-4.9	41.4	23.0	3.5	9.2	-19.8	-5.7	-7.1
-3.2	-29.2	.6	-6.6	45.0	9.7	26.0	-14.9
.0	-26.2	-1.0	-19.6	-11.7	7.1	-17.4	21.8
15.7	19.4	3.3	-7.0	-13.7	-21.9	4.0	3.7
-1.3							

Camera range = 50 cm

$s_{\min} = 2.50 \text{ \AA}^{-1}$ $s_{\max} = 14.00 \text{ \AA}^{-1}$ step size = $0.125 \text{ \AA}^{-1}$

				-252.7	-116.7	38.5	173.7
290.7	376.9	383.4	337.9	253.1	150.1	39.7	-43.0
-86.4	-103.2	-101.0	-107.0	-117.4	-160.4	-200.2	-239.7
-255.0	-234.1	-169.1	-60.1	61.6	191.0	294.3	342.3
335.8	276.9	184.5	89.8	9.6	-59.8	-91.8	-111.5
-114.3	-103.7	-115.1	-132.3	-160.6	-185.2	-186.0	-160.8

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-100.7	-21.7	73.6	160.0	211.1	249.7	246.2	207.8
154.0	74.4	12.3	-39.6	-79.6	-89.2	-102.9	-101.3
-111.9	-120.4	-126.4	-121.5	-115.0	-86.8	-51.8	10.9
59.2	101.8	149.1	166.0	163.6	140.9	96.7	56.1
13.5	-11.7	-45.7	-60.4	-70.2	-68.2	-84.6	-77.7
-93.6	-86.7	-85.0	-56.5	-28.0	0.4	43.8	75.4
105.3							

Vibrational amplitudes [$\text{\AA}$] of MgBr_2 (linear) and Mg_2Br_4 (D_{2h} symmetry) calculated from the computed frequencies at the MP2/Mg: QZ, Br: QZ-PP level (see the paper for details)

MgBr₂	
$l(\text{Mg}-\text{Br})$	0.091
$l(\text{Br}\cdots\text{Br})$	0.125
Mg₂Br₄	
$l(\text{Mg}-\text{Br}_t)$	0.088
$l(\text{Mg}-\text{Br}_b)$	0.144
$l(\text{Mg}\cdots\text{Mg})$	0.198
$l(\text{Br}_b\cdots\text{Br}_b)$	0.174
$l(\text{Mg}\cdots\text{Br}_t)$	0.214
$l(\text{Br}_b\cdots\text{Br}_t)$	0.306
$l(\text{Br}_t\cdots\text{Br}_t)$	0.231