

Figure 12.—Variation of lattice parameters with the ionic radius of LaSb<sub>2</sub>-type rare earth diantimonides.

TABLE II  
ΔH AND ΔS OF SEVERAL REACTIONS GIVING  
RARE EARTH DIANTIMONIDES

Reaction	ΔH, kcal/mol	ΔS, cal/mol deg
GdSb + Sb → GdSb <sub>2</sub> (LaSb <sub>2</sub> ) <sup>a</sup>	-7	-5
GdSb <sub>2</sub> (LaSb <sub>2</sub> ) → GdSb <sub>2</sub> (HPO) <sup>b</sup>	2	1
TbSb + Sb → TbSb <sub>2</sub> (LaSb <sub>2</sub> )	1	1
TbSb <sub>2</sub> (LaSb <sub>2</sub> ) → TbSb <sub>2</sub> (HPO)	1.5	1
DySb + Sb → DySb <sub>2</sub> (HPO)	6	4
HoSb + Sb → HoSb <sub>2</sub> (HPO)	3	2
ErSb + Sb → ErSb <sub>2</sub> (HPO)	4	3
TmSb + Sb → TmSb <sub>2</sub> (HPO)	7	4
YSb + Sb → YSb <sub>2</sub> (HPO)	4	3

<sup>a</sup> LaSb<sub>2</sub>-type structure. <sup>b</sup> High-pressure orthorhombic type.

check showed the bond lengths were calculated from the atomic positions given in Wang's dissertation. Apparently the atomic positions were refined after the dissertation was written but the bond lengths were not corrected. Corrected bond lengths were calculated using the atomic positions for SmSb<sub>2</sub> given in the published work. Figure 13 shows the variation of the shortest Sb-Sb bond length with ionic radius of the rare earth in the LaSb<sub>2</sub>-type rare earth diantimonides. It is apparent that the Sb-Sb bond can be as short as 2.76 Å and still be stable or at least metastable. This is 0.14 Å or almost 5% shorter than the bond length in anti-

TABLE III  
LATTICE PARAMETERS OF RARE EARTH DIANTIMONIDES

Di-antimonide	a, Å	b, Å	c, Å
LaSb <sub>2</sub> Type (Eight Molecules/Unit Cell)			
PrSb <sub>2</sub>	6.230 ± 0.006	6.063 ± 0.006	17.89 ± 0.02
NdSb <sub>2</sub>	6.230 ± 0.004	6.063 ± 0.004	17.89 ± 0.02
GdSb <sub>2</sub>	6.157 ± 0.002	5.986 ± 0.002	17.83 ± 0.01
TbSb <sub>2</sub>	6.123 ± 0.006	5.969 ± 0.006	17.72 ± 0.02
High-Pressure Orthorhombic Type (Two Molecules/Unit Cell)			
GdSb <sub>2</sub>	5.930 ± 0.003	3.296 ± 0.002	8.030 ± 0.004
TbSb <sub>2</sub>	5.903 ± 0.003	3.282 ± 0.002	7.990 ± 0.004
DySb <sub>2</sub>	5.888 ± 0.003	3.273 ± 0.002	7.965 ± 0.004
HoSb <sub>2</sub>	5.874 ± 0.002	3.266 ± 0.001	7.939 ± 0.003
ErSb <sub>2</sub>	5.866 ± 0.006	3.259 ± 0.003	7.926 ± 0.008
TmSb <sub>2</sub>	5.851 ± 0.002	3.252 ± 0.001	7.912 ± 0.004
YSb <sub>2</sub>	5.907 ± 0.003	3.283 ± 0.002	7.981 ± 0.004

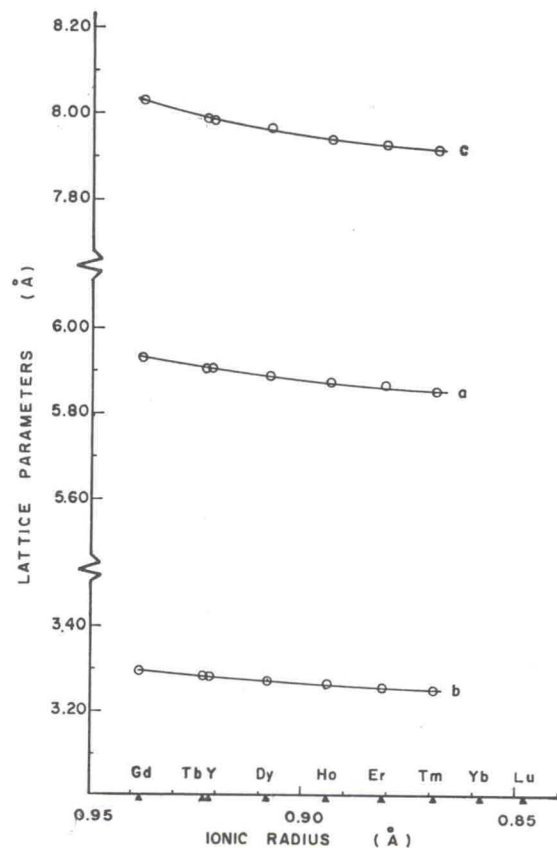


Figure 13.—Variation of lattice parameters with the ionic radius of high pressure orthorhombic type rare earth diantimonides.

mony metal which represents a considerable compression of the Sb-Sb bond. Assuming a Lennard-Jones 6-12 potential between the Sb atoms this represents a 5.4-kcal/mol strain on the Sb-Sb bond which is about 12% of the total bond energy.

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