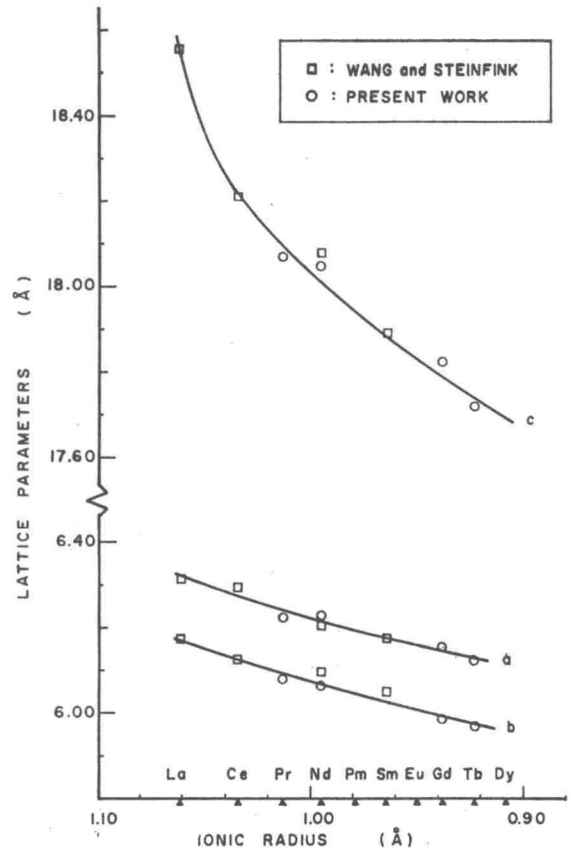

Figure 12.—Variation of lattice parameters with the ionic radius of $LaSb_2$-type rare earth diantimonides.

TABLE II

ΔH AND ΔS OF SEVERAL REACTIONS GIVING RARE EARTH DIANTIMONIDES

Reaction	ΔH, kcal/mol	ΔS, cal/mol deg
$GdSb + Sb \rightarrow GdSb_2$ $(LaSb_2)$[a]	−7	−5
$GdSb_2$ $(LaSb)_2 \rightarrow GdSb_2$ (HPO)[b]	2	1
$TbSb + Sb \rightarrow TbSb_2$ $(LaSb_2)$	1	1
$TbSb_2$ $(LaSb_2) \rightarrow TbSb_2$ (HPO)	1.5	1
$DySb + Sb \rightarrow DySb_2$ (HPO)	6	4
$HoSb + Sb \rightarrow HoSb_2$ (HPO)	3	2
$ErSb + Sb \rightarrow ErSb_2$ (HPO)	4	3
$TmSb + Sb \rightarrow TmSb_2$ (HPO)	7	4
$YSb + Sb \rightarrow YSb_2$ (HPO)	4	3

[a] $LaSb_2$-type structure. [b] 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 $SmSb_2$ 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 $LaSb_2$-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 antimony 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.

TABLE III

LATTICE PARAMETERS OF RARE EARTH DIANTIMONIDES

Diantimonide	a, Å	b, Å	c, Å
$LaSb_2$ Type (Eight Molecules/Unit Cell)			
$PrSb_2$	6.230 ± 0.006	6.063 ± 0.006	17.89 ± 0.02
$NdSb_2$	6.230 ± 0.004	6.063 ± 0.004	17.89 ± 0.02
$GdSb_2$	6.157 ± 0.002	5.986 ± 0.002	17.83 ± 0.01
$TbSb_2$	6.123 ± 0.006	5.969 ± 0.006	17.72 ± 0.02
High-Pressure Orthorhombic Type (Two Molecules/Unit Cell)			
$GdSb_2$	5.930 ± 0.003	3.296 ± 0.002	8.030 ± 0.004
$TbSb_2$	5.903 ± 0.003	3.282 ± 0.002	7.990 ± 0.004
$DySb_2$	5.888 ± 0.003	3.273 ± 0.002	7.965 ± 0.004
$HoSb_2$	5.874 ± 0.002	3.266 ± 0.001	7.939 ± 0.003
$ErSb_2$	5.866 ± 0.006	3.259 ± 0.003	7.926 ± 0.008
$TmSb_2$	5.851 ± 0.002	3.252 ± 0.001	7.912 ± 0.004
YSb_2	5.907 ± 0.003	3.283 ± 0.002	7.981 ± 0.004

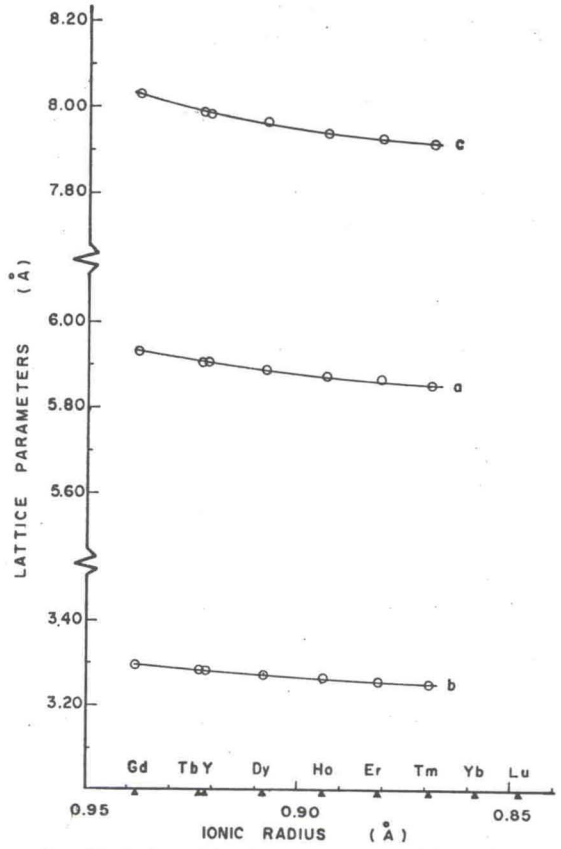

Figure 13.—Variation of lattice parameters with the ionic radius of high pressure orthorhombic type rare earth diantimonides.

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