

The ammonia borane tetramer

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Optimized geometry at the MP2/6-311++g(d,p) level

S4 structure

N	-2.40463400	0.07008600	0.81328800
H	-3.31786300	-0.04578500	1.24653200
H	-1.77149000	-0.63070300	1.20621500
B	-2.49881600	-0.07008600	-0.80079900
H	-1.36582000	0.07379100	-1.21698200
H	-2.90526700	-1.19139300	-1.03064000
H	-2.03202200	0.98185000	1.08808500
H	-3.24683000	0.79139000	-1.19703100
N	0.07008600	2.40463400	-0.81328800
H	0.98185000	2.03202200	-1.08808500
H	-0.63070300	1.77149000	-1.20621500
B	-0.07008600	2.49881600	0.80079900
H	-1.19139300	2.90526700	1.03064000
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