MNDO CALCULATION RESULTS

1SCF MNDO GEO-OK VECTORS BONDS
LiH

FINAL HEAT OF FORMATION = 26.97779 KCAL

TOTAL ENERGY = -19.78933 EV
ELECTRONIC ENERGY = -27.20810 EV
CORE-CORE REPULSION = 7.41878 EV

IONIZATION POTENTIAL = 8.38124
NO. OF FILLED LEVELS = 1
MOLECULAR WEIGHT = 7.948

ATOM NUMBER (I)	CHEMICAL SYMBOL	BOND LENGTH (ANGSTROMS) NA:I	BOND ANGLE (DEGREES) NB:NA:I	TWIST ANGLE (DEGREES) NC:NB:NA:I	NA	NB	NC
1	H						
2	Li	1.61000	*		1		

EIGENVECTORS

ROOT NO.		1	2	3	4	5
		-8.38124	.63258	2.45221	2.45221	5.60161
S	H 1	.84520	.15858	.00000	.00000	.51039
S	Li 2	.41231	-.80110	.00000	.00000	-.43387
PX	Li 2	-.34007	-.57714	.00000	.00000	.74247
PY	Li 2	.00000	.00000	.92376	-.38298	.00000
PZ	Li 2	.00000	.00000	.38298	.92376	.00000

NET ATOMIC CHARGES AND DIPOLE CONTRIBUTIONS

ATOM NO.	TYPE	CHARGE	ATOM ELECTRON DENSITY
1	H	-.4287	1.4287
2	Li	.4287	.5713

DIPOLE	X	Y	Z	TOTAL
POINT-CHG.	3.315	.000	.000	3.315
HYBRID	2.929	.000	.000	2.929
SUM	6.244	.000	.000	6.244

ATOMIC ORBITAL ELECTRON POPULATIONS

1.42871 .33999 .23130 .00000 .00000

BONDING CONTRIBUTION OF EACH M.O.

1.6324 -.1437 .0000 .0000 -1.4887

BOND ORDERS AND VALENCIES

		H 1	Li 2
H	1	.816209	
Li	2	.816209	.816209