NH_3 with fixed 90° bond angles HEAT OF FORMATION = 9.09266 KCAL

CARTESIAN COORDINATES	NO	ATOM	X	Y	Z
	1	H	0.0000	0.0000	0.0000
	2	N	1.0296	0.0000	0.0000
	3	H	1.0296	1.0296	0.0000
	4	H	1.0296	0.0000	-1.0296

EIGENVECTORS

ROOT NO.			1	2	3	4	5	6	7
ENERGY			-33.12	-15.03	-15.03	-12.01	4.59	4.78	4.78
S	H	1	-0.323	0.478	0.276	-0.231	-0.418	-0.300	0.520
S	N	2	-0.807	0.000	0.000	0.459	0.370	0.000	0.000
PX	N	2	0.105	-0.520	-0.300	0.457	-0.335	-0.276	0.478
PY	N	2	-0.105	0.000	-0.601	-0.457	0.335	-0.552	-0.000
PZ	N	2	0.105	0.520	-0.300	0.457	-0.335	-0.276	-0.478
S	H	3	-0.323	0.000	-0.552	-0.231	-0.418	0.601	0.000
S	H	4	-0.323	-0.478	0.276	-0.231	-0.418	-0.300	-0.520

BONDING CONTRIBUTION OF EACH M.O.

1.3341 1.9743 1.9743 0.6845 -1.9696 -1.9987 -1.9987

BOND-ORDER MATRIX			S-SIGMA H 1	S-SIGMA N 2	P-SIGMA N 2	S-SIGMA H 3	S-SIGMA H 4
S-SIGMA	H	1	0.994				
S-SIGMA	N	2	0.096	0.288			
P-SIGMA	N	2	0.893	0.000	2.679		
S-SIGMA	H	3	0.000	0.096	0.893	0.994	
S-SIGMA	H	4	0.000	0.096	0.893	0.000	0.994

NH_3 with 109° bond angles HEAT OF FORMATION = -7.28191 KCAL

CARTESIAN COORDINATES	NO.	ATOM	X	Y	Z
	1	H	0.0000	0.0000	0.0000
	2	N	0.9989	0.0000	0.0000
	3	H	1.3259	0.9425	0.0000
	4	H	1.3211	-0.4565	-0.8272

EIGENVECTORS

ROOT NO.			1	2	3	4	5	6	7
ENERGY			-32.68	-15.90	-15.88	-10.42	4.22	6.15	6.166
S	H	1	-0.313	0.310	0.462	0.158	-0.458	0.510	-0.307
S	N	2	-0.829	-0.000	0.000	-0.320	0.457	0.000	-0.000
PX	N	2	0.043	-0.38	-0.569	-0.308	-0.138	0.548	-0.331
PY	N	2	-0.061	-0.592	0.246	0.434	0.192	-0.201	-0.563
PZ	N	2	0.104	-0.189	0.386	-0.732	-0.325	-0.351	-0.194
S	H	3	-0.314	-0.555	0.037	0.159	-0.457	0.009	0.596
S	H	4	-0.314	0.245	-0.500	0.158	-0.456	-0.522	-0.289

BONDING CONTRIBUTION OF EACH M.O.

1.4127 2.0494 2.0485 0.3620 -2.0257 -1.9238 -1.9232

BOND ORDER MATRIX			S-SIGMA H 1	S-SIGMA N 2	P-SIGMA N 2	S-SIGMA H 3	S-SIGMA H 4
S-SIGMA	H	1	0.982				
S-SIGMA	N	2	0.175	0.526			
P-SIGMA	N	2	0.794	0.000	2.384		
S-SIGMA	H	3	0.003	0.175	0.794	0.982	
S-SIGMA	H	4	0.003	0.175	0.795	0.003	0.982