| NH3 with | rixea : | o Dona | angre | <u> </u> | ILAI OF | FORMAT. | LON = 9 | .09266 KCAL |
|--|--|--|--|--|---|--|--|---|
| | | COORDINA | | NO | ATOM | X | Y | <u>Z</u> |
| | | | | 1 | H | 0.0000 | 0.0000 | |
| | | | | 2 | | 1.0296 | 0.0000 | |
| | | | | 3 4 | | 1.0296 1.0296 | 1.0296 | |
| | | | | 4 | п | 1.0296 | 0.0000 | -1.0296 |
| | | EIGENVEC | | | | | | |
| ROOT NO. | | 2 | 3 | | 4 | 5_ | 6 | 7 |
| ENERGY | -33.12 | -15.03 | -15. | | -12.01 | | 4.78 | 4.78 |
| S H 1 | -0.323 | 0.478 | 0.2 | 76 | -0.231 | -0.41 | 8 -0.300 | 0.520 |
| | -0.807 | 0.000 | 0.0 | | 0.459 | | | |
| | 0.105 | -0.520 | -0.3 | | 0.457 | | | |
| | -0.105 | 0.000 0.520 | -0.6 | | -0.457 | | | |
| | 0.105 | | -0.3 | | 0.457 | | | |
| | -0.323 -0.323 | 0.000 -0.478 | -0.5 0.2 | | -0.231 -0.231 | | | |
| 5 11 4 | | DING CON | | | | | 0.500 | 0.520 |
| | 1.3341 | 1.9743 | 1.97 | | 0.6845 | | 6 -1.9987 | -1.9987 |
| BOND-ORD | ER MATR | IX S-SIGM | Δ ς | -ST(| GMA P-S | TGMA | S-SIGMA | S-STGMA |
| | | H 1 | | N 2 | | 2 | Н 3 | Н 4 |
| S-SIGM | А Н 1 | 0.994 | | | | | | |
| S-SIGM | | 0.096 | | .288 | | | | |
| P-SIGM | | 0.893 | | .000 | | | | |
| S-SIGM | | 0.000 | | .096 | | | 0.994 | 0 004 |
| S-SIGM | А Н 4 | 0.000 | U | .090 | 6 0.8 | 193 | 0.000 | 0.994 |
| | | | | | | | | |
| | | | | | | | | |
| | | | | | | | -7.281 | 91 KCAL |
| | | o <mark>nd angle</mark> OORDINATE | | NO | . ATOM | X | Y | Z |
| _ | | | | <u>NO</u> 1 | . ATOM H | X 0.0000 | 0.0000 | <u>z</u> |
| | | | | <u>NO</u> 1 2 | . ATOM H N | X 0.0000 0.9989 | 0.0000 0.0000 | Z 0.0000 0.0000 |
| | | | | NO 1 2 3 | H N H | X 0.0000 0.9989 1.3259 | Y 0.0000 0.0000 0.9425 | Z 0.0000 0.0000 0.0000 |
| | | | | <u>NO</u> 1 2 | H N H | X 0.0000 0.9989 | 0.0000 0.0000 | Z 0.0000 0.0000 0.0000 |
| _ | | OORDINATE EIGENVEC | S TORS | NO 1 2 3 | . ATOM H N H H | X 0.0000 0.9989 1.3259 1.3211 | Y 0.0000 0.0000 0.9425 -0.4565 | Z 0.0000 0.0000 0.0000 |
| CART | ESIAN CO | OORDINATE EIGENVEC 2 | S TORS 3 | NO 1 2 3 4 | H N H H | X 0.0000 0.9989 1.3259 1.3211 | Y 0.0000 0.0000 0.9425 -0.4565 | Z 0 0.0000 0 0.0000 6 0.0000 -0.8272 |
| CART: | 1 -32.68 | EIGENVEC 2 -15.90 | TORS 3 -15. | NO 1 2 3 4 | . ATOM H N H H | X 0.0000 0.9989 1.3259 1.3211 5 4.22 | Y 0.0000 0.0000 0.9425 -0.4565 | Z 0.0000 0.0000 6.0000 -0.8272 |
| CART: ROOT NO. ENERGY S H 1 | ESIAN CO | OORDINATE EIGENVEC 2 | TORS 3 -15. 0.4 | NO 1 2 3 4 88 62 | H N H H | X 0.0000 0.9989 1.3259 1.3211 5 4.22 | Y 0.0000 0.0000 0.9425 -0.4565 | Z 0 0.0000 0 0.0000 6 0.0000 6 -0.8272 7 6.166 0 -0.307 |
| CART. ROOT NO. ENERGY S H 1 S N 2 | 1 -32.68 -0.313 -0.829 | EIGENVEC 2 -15.90 0.310 -0.000 | TORS 3 -15. 0.4 0.0 | NO 1 2 3 4 88 62 00 | . ATOM H N H H -10.42 0.158 | X 0.0000 0.9989 1.3259 1.3211 5 4.22 4.22 6 -0.45 0.45 | Y 0.0000 0.9425 -0.4565 6 6.15 8 0.510 7 0.000 | Z 0.0000 0.0000 6.0000 60.8272 7 6.166 00.307 |
| ROOT NO. ENERGY S H 1 S N 2 PX N 2 | 1 -32.68 -0.313 -0.829 0.043 | EIGENVEC 2 -15.90 0.310 -0.000 -0.38 | TORS 3 -15. 0.4 0.0 -0.5 | NO 1 2 3 4 88 62 00 69 | . ATOM H N H H -10.42 0.158 -0.320 -0.308 | X 0.0000 0.9989 1.3259 1.3211 5 4.22 4.22 6 -0.45 0.45 -0.13 | Y 0.0000 0.9425 -0.4565 6 6.15 8 0.510 7 0.000 8 0.548 | Z 0.0000 0.0000 6.0000 6.0.8272 7 6.166 0.0.307 0.000 8.0.331 |
| ROOT NO. ENERGY S H 1 S N 2 PX N 2 PY N 2 | 1 -32.68 -0.313 -0.829 0.043 -0.061 | EIGENVEC 2 -15.90 0.310 -0.000 -0.38 -0.592 | TORS 3 -15. 0.4 0.0 -0.5 0.2 | NO 1 2 3 4 8 8 62 00 69 46 | . ATOM H N H H -10.42 0.158 -0.320 -0.308 0.434 | X 0.0000 0.9989 1.3259 1.3211 5 4.22 4.22 -0.45 0.45 -0.13 | Y 0.0000 0.9425 -0.4565 6 6.15 8 0.510 7 0.000 8 0.548 2 -0.201 | Z 0.0000 0.0000 6.0000 6.0.8272 7 6.166 0.0.307 0.000 8.0.331 -0.563 |
| ROOT NO. ENERGY S H 1 S N 2 PX N 2 PY N 2 PZ N 2 | 1 -32.68 -0.313 -0.829 0.043 -0.061 0.104 | EIGENVEC 2 -15.90 0.310 -0.000 -0.38 -0.592 -0.189 | TORS 3 -15. 0.4 0.0 -0.5 0.2 0.3 | NO 1 2 3 4 88 62 00 69 46 86 | . ATOM H N H -10.42 0.158 -0.320 -0.308 0.434 -0.732 | X 0.0000 0.9989 1.3259 1.3211 5 4.22 -0.45 0.45 -0.13 0.19 | Y 0.0000 0.9425 -0.4565 6 6.15 8 0.510 7 0.000 8 0.548 2 -0.201 5 -0.351 | Z 0 0.0000 0 0.0000 6 0.0000 6 -0.8272 7 6.166 0 -0.307 0 -0.000 8 -0.331 -0.563 -0.194 |
| CART: ROOT NO. ENERGY S H 1 S N 2 PX N 2 PX N 2 PY N 2 PZ N 2 S H 3 | 1 -32.68 -0.313 -0.829 0.043 -0.061 0.104 -0.314 | EIGENVEC 2 -15.90 0.310 -0.000 -0.38 -0.592 -0.189 -0.555 | TORS 3 -15. 0.4 0.0 -0.5 0.2 0.3 0.0 | NO 1 2 3 4 8 8 62 00 69 46 86 37 | . ATOM H N H -10.42 0.158 -0.320 -0.308 0.434 -0.732 0.159 | X 0.0000 0.9989 1.3259 1.3211 5 4.22 -0.45 0.45 -0.13 0.19 -0.32 -0.45 | Y 0.0000 0.9425 -0.4565 6 6.15 8 0.510 7 0.000 8 0.548 2 -0.201 5 -0.351 7 0.009 | 7 6.166 0 -0.307 0 -0.563 -0.194 0 .596 |
| CART: ROOT NO. ENERGY S H 1 S N 2 PX N 2 PX N 2 PY N 2 PZ N 2 S H 3 | 1 -32.68 -0.313 -0.829 0.043 -0.061 0.104 -0.314 -0.314 | EIGENVEC 2 -15.90 0.310 -0.000 -0.38 -0.592 -0.189 -0.555 0.245 | TORS 3 -15. 0.4 0.0 -0.5 0.2 0.3 0.0 -0.5 | NO 1 2 3 4 88 62 00 69 46 86 37 00 | . ATOM H N H H -10.42 0.158 -0.320 -0.308 0.434 -0.732 0.159 0.158 | X 0.0000 0.9989 1.3259 1.3211 5 4.22 -0.45 0.45 -0.13 0.19 -0.32 -0.45 -0.45 | Y 0.0000 0.9425 -0.4565 6 6.15 8 0.510 7 0.000 8 0.548 2 -0.201 5 -0.351 7 0.009 | 7 6.166 0 -0.307 0 -0.563 -0.194 0 .596 |
| CART: ROOT NO. ENERGY S H 1 S N 2 PX N 2 PX N 2 PY N 2 PZ N 2 S H 3 | 1 -32.68 -0.313 -0.829 0.043 -0.061 0.104 -0.314 -0.314 | EIGENVEC 2 -15.90 0.310 -0.000 -0.38 -0.592 -0.189 -0.555 | TORS 3 -15. 0.4 0.0 -0.5 0.2 0.3 0.0 -0.5 | 88 62 00 69 46 86 37 00 J OF | . ATOM H N H H -10.42 0.158 -0.320 -0.308 0.434 -0.732 0.159 0.158 | X 0.0000 0.9989 1.3259 1.3211 5 4.22 -0.45 0.45 -0.13 0.19 -0.32 -0.45 -0.45 | Y 0.0000 0.9425 -0.4565 6 6.15 8 0.510 7 0.000 8 0.548 2 -0.201 5 -0.351 7 0.009 6 -0.522 | Z 0.0000 0.0000 0.0000 6.0.8272 7 6.166 0.000 8.0.307 0.000 8.0.331 0.563 0.194 0.596 2.0.289 |
| ROOT NO. ENERGY S H 1 S N 2 PX N 2 PY N 2 PY N 2 PZ N 2 S H 3 S H 4 | 1 -32.68 -0.313 -0.829 0.043 -0.061 0.104 -0.314 -0.314 BONDING 1.4127 | EIGENVEC 2 -15.90 0.310 -0.000 -0.38 -0.592 -0.189 -0.555 0.245 G CONTRIB 2.0494 | TORS 3 -15. 0.4 0.0 -0.5 0.2 0.3 0.0 -0.5 | 88 62 00 69 46 86 37 00 VOF | . ATOM H N H H -10.42 0.158 -0.320 -0.308 0.434 -0.732 0.159 0.158 EACH M 0.3620 | X 0.0000 0.9989 1.3259 1.3211 5 4.22 -0.45 0.45 -0.13 0.19 -0.32 -0.45 -0.45 | Y 0.0000 0.9425 -0.4565 6 6.15 8 0.510 7 0.000 8 0.548 2 -0.201 5 -0.351 7 0.009 6 -0.522 7 -1.9238 | Z 0.0000 0.0000 0.0000 0.0000 -0.8272 7 6.166 0.000 3.07 0.000 3.0.331 -0.563 -0.194 0.596 2.0.289 3.1.9232 |
| ROOT NO. ENERGY S H 1 S N 2 PX N 2 PY N 2 PY N 2 PZ N 2 S H 3 S H 4 | 1 -32.68 -0.313 -0.829 0.043 -0.061 0.104 -0.314 -0.314 BONDING 1.4127 | EIGENVEC 2 -15.90 0.310 -0.000 -0.38 -0.592 -0.189 -0.555 0.245 G CONTRIB | TORS 3 -15. 0.4 0.00 -0.5 0.2 0.3 0.0 -0.5 UTION 2.04 | 88 62 00 69 46 86 37 00 VOF | . ATOM H N H H -10.42 0.158 -0.320 -0.308 0.434 -0.732 0.159 0.158 EACH M 0.3620 | X 0.0000 0.9989 1.3259 1.3211 5 4.22 -0.45 0.45 -0.13 -0.32 -0.45 -0.45 | Y 0.0000 0.9425 -0.4565 6 6.15 8 0.510 7 0.000 8 0.548 2 -0.201 5 -0.351 7 0.009 6 -0.522 7 -1.9238 | Z 0.0000 0.0000 0.0000 0.0000 -0.8272 7 6.166 0.000 3.07 0.000 3.0.331 -0.563 -0.194 0.596 2.0.289 3.1.9232 |
| ROOT NO. ENERGY S H 1 S N 2 PX N 2 PY N 2 PY N 2 PZ N 2 S H 3 S H 4 | 1 -32.68 -0.313 -0.829 0.043 -0.061 0.104 -0.314 -0.314 BONDING 1.4127 | EIGENVEC 2 -15.90 0.310 -0.000 -0.38 -0.592 -0.189 -0.555 0.245 G CONTRIB 2.0494 IX S-SIGM | TORS 3 -15. 0.4 0.00 -0.5 0.2 0.3 0.0 -0.5 UTION 2.04 | 88 62 00 69 46 86 37 00 VOF | . ATOM H N H H -10.42 0.158 -0.320 -0.308 0.434 -0.732 0.159 0.158 EACH M 0.3620 | X 0.0000 0.9989 1.3259 1.3211 5 4.22 -0.45 0.45 -0.13 0.19 -0.32 -0.45 -0.45 | Y 0.0000 0.9425 -0.4565 6 6.15 8 0.510 7 0.000 8 0.548 2 -0.201 5 -0.351 7 0.009 6 -0.522 7 -1.9238 S-SIGMA | Z 0 0.0000 0 0.0000 6 0.0000 6 0.0000 6 -0.8272 7 6.166 0 -0.307 0 -0.000 8 -0.331 1 -0.563 1 -0.194 0 0.596 2 -0.289 8 -1.9232 S-SIGMA |
| ROOT NO. ENERGY S H 1 S N 2 PX N 2 PY N 2 PZ N 2 S H 3 S H 4 BOND ORD: S-SIGM. S-SIGM. | 1 -32.68 -0.313 -0.829 0.043 -0.061 0.104 -0.314 BONDING 1.4127 ER MATRI | EIGENVEC 2 -15.90 0.310 -0.000 -0.38 -0.592 -0.189 -0.555 0.245 G CONTRIB 2.0494 IX S-SIGM H 1 0.982 0.175 | TORS 3 -15. 0.4 0.00 -0.5 0.2 0.3 0.0 -0.5 UTION 2.04 | 88 62 00 69 46 86 37 00 1 OF | . ATOM H N H H -10.42 0.158 -0.320 -0.308 0.434 -0.732 0.159 0.158 EACH M 0.3620 GMA P-S 2 N | X 0.0000 0.9989 1.3259 1.3211 5 4.22 -0.45 0.45 -0.13 0.19 -0.32 -0.45 -0.45 .O. -2.025 | Y 0.0000 0.9425 -0.4565 6 6.15 8 0.510 7 0.000 8 0.548 2 -0.201 5 -0.351 7 0.009 6 -0.522 7 -1.9238 S-SIGMA | Z 0 0.0000 0 0.0000 6 0.0000 6 0.0000 6 -0.8272 7 6.166 0 -0.307 0 -0.000 8 -0.331 1 -0.563 1 -0.194 0 0.596 2 -0.289 8 -1.9232 S-SIGMA |
| CART: ROOT NO. ENERGY S H 1 S N 2 PX N 2 PY N 2 PZ N 2 S H 3 S H 4 BOND ORD: S-SIGM. S-SIGM. P-SIGM. | 1 -32.68 -0.313 -0.829 0.043 -0.061 0.104 -0.314 BONDING 1.4127 ER MATRI | EIGENVEC 2 -15.90 0.310 -0.000 -0.38 -0.592 -0.189 -0.555 0.245 G CONTRIB 2.0494 IX S-SIGM H 1 0.982 0.175 0.794 | TORS 3 -15. 0.4 0.00 -0.5 0.2 0.3 0.0 -0.5 UTION 2.04 | 88 62 00 69 46 86 37 00 1 OF -SIC .000 | . ATOM H N H H -10.42 0.158 -0.320 -0.308 0.434 -0.732 0.159 0.158 EACH M 0.3620 | X 0.0000 0.9989 1.3259 1.3211 5 4.22 -0.45 0.45 -0.13 0.19 -0.32 -0.45 -0.45 .O. -2.025 | Y 0.0000 0.9425 -0.4565 6 6.15 8 0.510 7 0.000 8 0.548 2 -0.201 5 -0.351 7 0.009 6 -0.522 7 -1.9238 S-SIGMA H 3 | Z 0 0.0000 0 0.0000 6 0.0000 6 0.0000 6 -0.8272 7 6.166 0 -0.307 0 -0.000 8 -0.331 1 -0.563 1 -0.194 0 0.596 2 -0.289 8 -1.9232 S-SIGMA |
| ROOT NO. ENERGY S H 1 S N 2 PX N 2 PY N 2 PZ N 2 S H 3 S H 4 BOND ORD: S-SIGM. S-SIGM. | 1 -32.68 -0.313 -0.829 0.043 -0.061 0.104 -0.314 BONDING 1.4127 ER MATRE | EIGENVEC 2 -15.90 0.310 -0.000 -0.38 -0.592 -0.189 -0.555 0.245 G CONTRIB 2.0494 IX S-SIGM H 1 0.982 0.175 | TORS 3 -15. 0.4 0.0 -0.5 0.2 0.3 0.0 -0.5 UTION 2.04 | 88 62 00 69 46 86 37 00 1 OF | . ATOM H N H H2 -10.42 0.158 -0.320 -0.308 0.434 -0.732 0.159 0.158 EACH M 0.3620 GMA P-S 2 N | X 0.0000 0.9989 1.3259 1.3211 5 4.22 -0.45 0.45 -0.13 0.19 -0.32 -0.45 -0.45 .O. -2.025 | Y 0.0000 0.9425 -0.4565 6 6.15 8 0.510 7 0.000 8 0.548 2 -0.201 5 -0.351 7 0.009 6 -0.522 7 -1.9238 S-SIGMA | Z 0 0.0000 0 0.0000 6 0.0000 6 0.0000 6 -0.8272 7 6.166 0 -0.307 0 -0.000 8 -0.331 1 -0.563 1 -0.194 0 0.596 2 -0.289 8 -1.9232 S-SIGMA |