

Linear CO₂, MNDO: O₁—C₂—O₃

| CARTESIAN COORDINATES | | | | |
|-----------------------|------|--------|-------|-------|
| NO. | ATOM | X | Y | Z |
| 1 | O | .0000 | .0000 | .0000 |
| 2 | C | 1.1806 | .0000 | .0000 |
| 3 | O | 2.3720 | .0000 | .0000 |

| ROOT NO. | | 1 | 2 | 3 | 4 | 5 | 6 |
|----------|-----|-----------|-----------|-----------|-----------|-----------|-----------|
| | | -45.57706 | -42.64601 | -21.24505 | -17.81440 | -17.68225 | -17.68225 |
| S | O 1 | -.54648 | .60628 | -.42030 | -.31273 | .00000 | .00000 |
| PX | O 1 | -.18114 | .15245 | .43326 | .54660 | .00000 | .00000 |
| PY | O 1 | .00000 | .00000 | .00000 | .00000 | -.09341 | -.55288 |
| PZ | O 1 | .00000 | .00000 | .00000 | .00000 | .55288 | -.09341 |
| S | C 2 | -.58061 | .00000 | .52083 | .00000 | .00000 | .00000 |
| PX | C 2 | .00000 | -.46730 | .00000 | -.45482 | .00000 | .00000 |
| PY | C 2 | .00000 | .00000 | .00000 | .00000 | -.10150 | -.60075 |
| PZ | C 2 | .00000 | .00000 | .00000 | .00000 | .60075 | -.10150 |
| S | O 3 | -.54648 | -.60628 | -.42030 | .31273 | .00000 | .00000 |
| PX | O 3 | .18114 | .15245 | -.43326 | .54660 | .00000 | .00000 |
| PY | O 3 | .00000 | .00000 | .00000 | .00000 | -.09341 | -.55288 |
| PZ | O 3 | .00000 | .00000 | .00000 | .00000 | .55288 | -.09341 |
| ROOT NO. | | 7 | 8 | 9 | 10 | 11 | 12 |
| | | -12.79386 | -12.79386 | .85052 | .85052 | 3.18416 | 7.94193 |
| S | O 1 | .00000 | .00000 | .00000 | .00000 | .15721 | .18609 |
| PX | O 1 | .00000 | .00000 | .00000 | .00000 | .52865 | .42189 |
| PY | O 1 | .27249 | -.65249 | -.42035 | .09437 | .00000 | .00000 |
| PZ | O 1 | -.65249 | -.27249 | -.09437 | -.42035 | .00000 | .00000 |
| S | C 2 | .00000 | .00000 | .00000 | .00000 | -.62580 | .00000 |
| PX | C 2 | .00000 | .00000 | .00000 | .00000 | .00000 | .75814 |
| PY | C 2 | .00000 | .00000 | .77371 | -.17369 | .00000 | .00000 |
| PZ | C 2 | .00000 | .00000 | .17369 | .77371 | .00000 | .00000 |
| S | O 3 | .00000 | .00000 | .00000 | .00000 | .15721 | -.18609 |
| PX | O 3 | .00000 | .00000 | .00000 | .00000 | -.52865 | .42189 |
| PY | O 3 | -.27249 | .65249 | -.42035 | .09437 | .00000 | .00000 |
| PZ | O 3 | .65249 | .27249 | -.09437 | -.42035 | .00000 | .00000 |

SIGMA-PI BOND-ORDER MATRIX

| | | S-SIGMA | P-SIGMA | P-PI | S-SIGMA | P-SIGMA | P-PI | S-SIGMA | P-SIGMA | P-PI |
|---------|-----|---------|---------|--------|---------|---------|--------|---------|---------|--------|
| | | O 1 | O 1 | O 1 | C 2 | C 2 | C 2 | O 3 | O 3 | O 3 |
| S-SIGMA | O 1 | .1188 | | | | | | | | |
| P-SIGMA | O 1 | .0000 | .8883 | | | | | | | |
| P-PI | O 1 | .0000 | .0000 | 1.2093 | | | | | | |
| S-SIGMA | C 2 | .0387 | .4378 | .0000 | .9530 | | | | | |
| P-SIGMA | C 2 | .0796 | .4092 | .0000 | .0000 | .9776 | | | | |
| P-PI | C 2 | .0000 | .0000 | .9336 | .0000 | .0000 | 1.8673 | | | |
| S-SIGMA | O 3 | .0004 | .0001 | .0000 | .0387 | .0796 | .0000 | .1188 | | |
| P-SIGMA | O 3 | .0001 | .0412 | .0000 | .4378 | .4092 | .0000 | .0000 | .8883 | |
| P-PI | O 3 | .0000 | .0000 | .2756 | .0000 | .0000 | .9336 | .0000 | .0000 | 1.2092 |

BOND ORDERS AND VALENCIES

| | | O1 | C2 | O3 |
|---|---|---------|---------|---------|
| O | 1 | 2.21633 | | |
| C | 2 | 1.89898 | 3.79796 | |
| O | 3 | .31735 | 1.89898 | 2.21633 |