Linear Triplet Ozone, MNDO: O₁— O₂ — O₃

		ROOT NO.	1	2	3	4	5	6
			-49.19162	-42.56203	-28.63517	-21.55537	-19.19295	-19.19295
S	O	1	-.40657	.58558	.57371	.36981	.00000	.00000
PX	O	1	-.19859	.18022	-.22397	-.47503	.00000	.00000
PY	O	1	.00000	.00000	.00000	.00000	.22954	.38991
PZ	O	1	.00000	.00000	.00000	.00000	-.38991	.22954
S	O	2	-.76846	.00001	-.49131	.00000	.00000	.00000
PX	O	2	-.00001	-.49925	.00000	.52456	.00000	.00000
PY	O	2	.00000	.00000	.00000	.00000	.38986	.66224
PZ	O	2	.00000	.00000	.00000	.00000	-.66224	.38986
S	O	3	-.40658	-.58557	.57371	-.36981	.00000	.00000
PX	O	3	.19859	.18022	.22398	-.47503	.00000	.00000
PY	O	3	.00000	.00000	.00000	.00000	.22955	.38992
PZ	O	3	.00000	.00000	.00000	.00000	-.38992	.22955

		ROOT NO.	7	8	9	10	11	12
			-13.16228	-13.16228	-6.32936	-6.32936	-.09863	8.94886
S	O	1	.00000	.00000	.00000	.00000	.07455	.14262
PX	O	1	.00000	.00000	.00000	.00000	.64062	.49180
PY	O	1	.70709	.00532	.33505	.42780	.00000	.00000
PZ	O	1	-.00532	.70709	.42780	-.33505	.00000	.00000
S	O	2	.00000	.00000	.00000	.00000	-.40999	.00000
PX	O	2	.00000	.00000	.00000	.00000	.00000	.68963
PY	O	2	.00000	.00000	-.39455	-.50377	.00000	.00000
PZ	O	2	.00000	.00000	-.50377	.39455	.00000	.00000
S	O	3	.00000	.00000	.00000	.00000	.07455	-.14263
PX	O	3	.00000	.00000	.00000	.00000	-.64062	.49180
PY	O	3	-.70708	-.00532	.33506	.42780	.00000	.00000
PZ	O	3	.00532	-.70708	.42780	-.33506	.00000	.00000

$$O_3$$
$$|$$

90° Bent Singlet Ozone, MNDO: O₁ — O₂

		ROOT NO.	1	2	3	4	5	6
			-50.96759	-37.77971	-30.58257	-20.60473	-20.28767	-18.93514
S	O	1	-.42472	.63547	.50507	-.29225	.23159	.00000
PX	O	1	-.22130	.11644	-.11563	.43944	-.36672	.00000
PY	O	1	-.02992	-.06006	.05467	-.14534	-.25456	.00000
PZ	O	1	.00000	.00000	.00000	.00000	.00000	-.42522
S	O	2	-.69423	.00000	-.63197	.00000	.20472	.00000
PX	O	2	.16960	-.28109	-.16985	-.44761	.47553	.00000
PY	O	2	-.16960	-.28109	.16985	-.44761	-.47553	.00000
PZ	O	2	.00000	.00000	.00000	.00000	.00000	-.79899
S	O	3	-.42472	-.63547	.50507	.29225	.23159	.00000
PX	O	3	.02992	-.06006	-.05467	-.14534	.25456	.00000
PY	O	3	.22130	.11644	.11563	.43944	.36672	.00000
PZ	O	3	.00000	.00000	.00000	.00000	.00000	-.42522

		ROOT NO.	7	8	9	10	11	12
			-14.14099	-12.37648	-12.18767	-2.82343	3.69998	3.82012
S	O	1	.02222	.00000	.00550	.00000	-.10361	.10192
PX	O	1	-.17469	.00000	.16226	.00000	-.51672	.52216
PY	O	1	.65553	.00000	.68498	.00000	.07796	.03995
PZ	O	1	.00000	-.70711	.00000	-.56497	.00000	.00000
S	O	2	.11585	.00000	.00000	.00000	.00000	-.25163
PX	O	2	.18045	.00000	-.06670	.00000	-.46496	.42860
PY	O	2	-.18045	.00000	-.06670	.00000	-.46496	-.42860
PZ	O	2	.00000	.00000	.00000	.60135	.00000	.00000
S	O	3	.02222	.00000	-.00550	.00000	.10361	.10192
PX	O	3	-.65553	.00000	.68498	.00000	.07796	-.03995
PY	O	3	.17469	.00000	.16226	.00000	-.51672	-.52216
PZ	O	3	.00000	.70711	.00000	-.56497	.00000	.00000