

B3LYP/6-31+G(d) computed energies and zero-point energies (zpe) are given in hartrees. The standard orientation (xyz) coordinates also are provided.

$\text{C}_6\text{H}_5\text{CO}_2$ Radical

E = -420.16932

zpe = 0.101848

H	.000000	2.152839	-.105681
C	.000000	1.217887	.447516
C	.000000	-1.214411	1.841749
C	.000000	.000000	-.247802
C	.000000	1.214411	1.841749
C	.000000	.000000	2.537278
C	.000000	-1.217887	.447516
C	.000000	.000000	-1.720595
H	.000000	2.154742	2.385827
H	.000000	.000000	3.624175
H	.000000	-2.152839	-.105681
H	.000000	-2.154742	2.385827
O	.000000	-1.042947	-2.441809
O	.000000	1.042947	-2.441809

$\text{C}_6\text{H}_5\text{CO}_2^-$

E = -420.29548

zpe = 0.101868

H	.000000	2.127742	-.135011
C	.000000	1.204340	.437783
C	.000000	-1.208734	1.836756
C	.000000	.000000	-.280915
C	.000000	1.208734	1.836756
C	.000000	.000000	2.543905
C	.000000	-1.204340	.437783
C	.000000	.000000	-1.833379
H	.000000	2.154102	2.379427
H	.000000	.000000	3.633391
H	.000000	-2.127742	-.135011
H	.000000	-2.154102	2.379427
O	.000000	-1.137806	-2.374648
O	.000000	1.137806	-2.374648

***m*-PyrCO₂ Radical**

E = -436.20263

zpe = 0.089921

H	2.161385	.167749	.000000
C	1.242267	-.411770	.000000
N	-1.159405	-1.876933	.000000
C	.000000	.234943	.000000
C	-1.258954	-1.802939	.000000
C	.036373	-2.484239	.000000
C	-1.168683	-.540964	.000000
C	-.078459	1.705644	.000000
H	.014271	-3.572187	.000000
H	-2.144985	-.061251	.000000
O	.926951	2.475081	.000000
O	-1.158409	2.369268	.000000
H	2.194116	-2.354626	.000000

***m*-PyrCO₂⁻**

E = -436.33858

zpe = 0.090316

H	2.133723	.175250	.000000
C	1.220577	-.414157	.000000
N	-1.183471	-1.860274	.000000
C	.000000	.267450	.000000
C	1.228077	-1.811612	.000000
C	.004290	-2.485054	.000000
C	-1.164971	-.514519	.000000
C	-.058721	1.817183	.000000
H	-.028344	-3.575673	.000000
H	-2.126712	-.008458	.000000
O	1.061247	2.393167	.000000
O	-1.215066	2.313006	.000000
H	2.160665	-2.374330	.000000

1R

E = -664.05062

zpe = 0.130508

H	-.000613	2.040428	.000000
C	.000000	.955036	.000000
N	.008429	-1.807046	.000000
C	.001887	.249236	1.209062
C	.001887	.249236	-1.209062
C	.005525	-1.136350	-1.177693
C	.005525	-1.136350	1.177693
C	.003824	.936580	2.566583
C	.003824	.936580	-2.566583
H	.007248	-1.719290	-2.091916
H	.007248	-1.719290	2.091916
O	-.002252	2.190650	2.594227
O	.010743	.208023	3.588533
O	-.002252	2.190650	-2.594227
O	.010743	.208023	-3.588533
H	-1.076642	-3.619341	.000000
H	.472481	-3.657939	.890632
H	.472481	-3.657939	-.890632
C	-.035316	-3.286647	.000000

1

E = -664.21423

zpe = 0.132664

H	-0.003165	2.045821	0.000000
C	0.000000	0.959997	0.000000
N	0.009770	-1.790905	0.000000
C	0.003834	0.265406	1.220009
C	0.003834	0.265406	-1.220009
C	0.007505	-1.119127	-1.180562
C	0.007505	-1.119127	1.180562
C	0.005044	0.950365	2.621158
C	0.005044	0.950365	-2.621158
H	0.010668	-1.690168	-2.102294
H	0.010668	-1.690168	2.102294
O	-0.008477	2.198342	2.598482
O	0.018466	0.138582	3.584209
O	-0.008477	2.198342	-2.598482
O	0.018466	0.138582	-3.584209
H	-1.087240	-3.596335	0.000000
H	0.458090	-3.639437	0.891411
H	0.458090	-3.639437	-0.891411
C	-0.045322	-3.260740	0.000000

2R

E = -664.08781

zpe = 0.132734

H	-0.725751	1.514203	0.000000
C	0.000000	0.706011	0.000000
N	1.860805	-1.402642	0.000000
C	1.373449	0.957766	0.000000
C	-0.430328	-0.621925	0.000000
C	0.541622	-1.636083	0.000000
C	2.262325	-0.128525	0.000000
C	1.886720	2.340308	0.000000
C	-1.898481	-0.900923	0.000000
H	0.240257	-2.679209	0.000000
H	3.336527	0.042255	0.000000
O	1.154944	3.373335	0.000000
O	3.114386	2.648537	0.000000
O	-2.749756	-0.033430	0.000000
O	-2.168727	-2.220137	0.000000
C	-3.566717	-2.578714	0.000000
H	-4.056746	-2.182145	0.892527
H	-3.581493	-3.668389	0.000000
H	-4.056746	-2.182145	-0.892527

2

E = -664.22959

zpe = 0.133053

H	-0.713927	1.544627	0.000000
C	0.000000	0.726713	0.000000
N	1.873466	-1.364396	0.000000
C	1.363832	1.018113	0.000000
C	-0.421024	-0.613137	0.000000
C	0.561128	-1.619195	0.000000
C	2.248051	-0.070027	0.000000
C	1.887498	2.479965	0.000000
C	-1.868144	-0.925434	0.000000
H	0.272813	-2.667133	0.000000
H	3.315205	0.134222	0.000000
O	0.994173	3.363673	0.000000
O	3.140029	2.595010	0.000000
O	-2.774293	-0.110498	0.000000
O	-2.119305	-2.271186	0.000000
C	-3.502344	-2.638231	0.000000
H	-4.006954	-2.249683	0.890095
H	-3.513251	-3.730158	0.000000
H	-4.006954	-2.249683	-0.890095

3R

E = -475.45798

zpe = 0.117898

H	-1.230227	2.239144	.010411
C	-.383331	1.556241	.002613
N	1.704988	-.303647	-.012683
C	.947804	1.922172	-.004780
C	-.644523	.177571	-.001433
C	.416138	-.720677	-.008105
C	1.989283	1.034341	-.012570
C	2.808352	-1.286354	.022743
C	-2.130570	-.376297	.000967
H	.219273	-1.786650	-.010973
H	3.038486	1.309644	-.019408
H	2.425324	-2.258897	-.286138
H	3.206982	-1.354154	1.038670
O	-2.993798	.512870	.021213
O	-2.157362	-1.624698	-.018174
H	3.595595	-.970922	-.664703

3

E = -475.55756

zpe = 0.117209

H	-1.113198	2.248838	0.068617
C	-0.279116	1.548621	0.024252
N	1.674344	-0.346889	-0.024129
C	1.062270	2.036274	-0.004653
C	-0.642840	0.190103	-0.004593
C	0.381161	-0.745556	-0.014728
C	1.989326	1.000822	-0.034533
C	2.736419	-1.355695	0.042424
C	-2.106367	-0.334875	-0.002456
H	0.163201	-1.808094	-0.011434
H	3.068855	1.165602	-0.075515
H	2.411365	-2.265918	-0.467755
H	2.975699	-1.595180	1.085112
O	-2.999047	0.544643	0.022489
O	-2.213999	-1.593033	-0.024434
H	3.632921	-0.968048	-0.448841