

M062x/6-311++G**

CH₄-CO₂

C	0.9546619500	-0.0249674461	-0.1882548655
O	0.9633531698	1.1238985572	-0.3058392756
O	0.9513274625	-1.1739178858	-0.0711378784
H	-1.8425356482	0.9252533705	0.5530711187
C	-2.2622995462	0.0205557841	0.1141111464
H	-1.8700656552	-0.8586655251	0.6242958723
H	-2.0054506884	-0.0249928921	-0.9443318867
H	-3.3462260267	0.0416947182	0.2171017976

CH₄-(CO₂)₂

C	-1.6990947010	0.5326766770	0.2352041425
O	-2.3892377786	0.2611398644	-0.6477159435
O	-1.0134790626	0.8044811675	1.1267646249
C	1.6065743032	0.5287536604	-0.2507230416
O	2.3442467138	0.4079074981	0.6272449432
O	0.8724517278	0.6499755356	-1.1368526438
H	-0.1932908843	-3.3138806324	0.3136513931
C	0.1660708702	-2.3224571942	0.0420177026
H	-0.4829626378	-1.9009012455	-0.7255403042
H	1.1804266793	-2.4065207728	-0.3484431613
H	0.1689057864	-1.6896742557	0.9304291159

CH₄-(CO₂)₃

C	1.0990887526	1.5718306766	0.7751862097
O	0.9978698433	0.5515397506	1.3123335456
O	1.2158788582	2.5903702572	0.2486384299
C	-2.3621442201	0.4265604884	-0.1842749697
O	-3.2779481178	-0.2652495573	-0.0822497267
O	-1.4552166124	1.1382438753	-0.2899757966
C	0.5093589869	-2.0247363429	0.3043343205
O	-0.5737729527	-1.7031382965	0.0548913606
O	1.5842650616	-2.3641438215	0.5461246609
H	2.0197873026	0.9693152369	-2.4401333521
C	1.6765545029	0.0550805946	-1.9581166574
H	2.3452877772	-0.1948595644	-1.1333919338
H	1.6841369961	-0.7603377753	-2.6809454404
H	0.6596557753	0.2038132797	-1.5924894330

CH₄-(CO₂)₄

C	-0.1815388300	1.3159690720	1.6297762927
O	0.3012316244	0.2622963676	1.6330758070
O	-0.6617325158	2.3623758784	1.6428984354
C	-1.2031136959	0.3216389403	-1.8086662476
O	-1.9002136297	-0.2831578488	-2.4968796028
O	-0.5057518102	0.9520287613	-1.1307184880
C	0.2632240975	-2.2894568068	0.4117980810
O	-0.5435803386	-1.9176627789	-0.3305398950
O	1.0549167279	-2.6802257038	1.1523670497
C	2.2102876330	0.5653743918	-0.4570004161
O	2.3091886807	1.6594267909	-0.1022653982
O	2.1207951409	-0.5299661741	-0.8147098385
H	-2.8165083474	0.9192249036	0.5661573152
C	-3.1118990648	-0.0889927747	0.8598859276
H	-4.1133394697	-0.0517877414	1.2862227849
H	-2.4174448871	-0.4789991367	1.6042813624
H	-3.1116500712	-0.7495962817	-0.0065135025

CH₄-(CO₂)₅

C	-3.1363067303	-0.0171679368	0.0887064352
O	-2.4773965307	-0.0494668926	-0.8641479979
O	-3.8081593024	0.0229175269	1.0226967999
C	2.7884723126	0.8907273511	0.0552422862
O	3.3980842633	-0.0876752129	-0.0003462233
O	2.1908374020	1.8790714304	0.1012916836
C	-0.5586181986	2.2107577477	-0.3526990173
O	-0.3532462633	2.6011777985	-1.4169630702
O	-0.7912259107	1.8268749704	0.7151761486
C	0.0470368057	-0.6257385303	1.7881461997
O	1.0977183143	-0.2077148006	2.0178794227
O	-1.0010327815	-1.0616603729	1.5676046381
C	-0.0152558047	-1.1006482971	-1.6872090493
O	-0.4927049806	-1.8638770455	-2.4030826611
O	0.4787489180	-0.3341854383	-0.9698967016
H	0.3818120408	-3.1356820151	0.3761422854
C	1.4414585839	-3.2532364026	0.1432381401
H	1.8430190936	-4.0764686909	0.7324192472
H	1.9907327580	-2.3413397044	0.3777123463
H	1.5557195938	-3.4868197527	-0.9155370925

CH₃F-CO₂

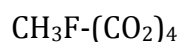
C	1.3563338564	-0.1611540041	0.0103418421
O	1.8202750024	0.8944267451	-0.0088357824
O	0.9218086436	-1.2333411449	0.0299164341
H	-2.7547783078	-0.0904220621	0.8852299727
C	-2.1481573966	-0.2483785226	-0.0060117038
H	-2.7510490592	-0.1187220890	-0.9043113477
H	-1.6911776277	-1.2374910274	0.0107171600
F	-1.1334512716	0.6994265318	-0.0189140169

CH₃F-(CO₂)₂

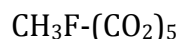
C	1.2747285138	-1.1914637313	0.0727070268
O	2.0859071389	-0.6006361061	0.6450606624
O	0.4738655470	-1.8018384197	-0.4932583560
C	-1.8042128234	-0.1554373477	0.2397658768
O	-2.3968380777	-0.2742373576	-0.7408258824
O	-1.2310985031	-0.0372381013	1.2397143636
H	1.9529569287	2.1035677400	-0.0588912557
C	0.8691256062	2.1434964562	0.0364797745
H	0.4842254977	3.1058369120	-0.2982384846
H	0.5693791722	1.9386515062	1.0638185374
F	0.3231746393	1.1528355662	-0.7787007663

CH₃F-(CO₂)₃

C	-0.1114031789	-2.0615866970	-0.1394085750
O	-1.0291052234	-2.3637734956	0.4946134135
O	0.8152799071	-1.7850457033	-0.7705754805
C	2.0469843711	0.7746167216	-0.4808129634
O	1.2643112277	1.2264607142	-1.2021961171
O	2.8457734452	0.3439746164	0.2316835192
C	-1.5325846409	1.1032896343	-0.8719953188
O	-1.5084097362	0.0669186600	-1.3822501747
O	-1.5909253906	2.1378247478	-0.3620089696
H	-1.3835875031	-0.4434878719	2.4664423791
C	-0.6905278759	0.3901694134	2.3592446194
H	0.0433524436	0.3915066379	3.1632560833
H	-1.2211144522	1.3402994877	2.3148077013
F	-0.0086087319	0.2240889154	1.1512896639



C	-0.1144882953	-1.9594400636	-0.1800226442
O	-1.0626419225	-1.9684766251	-0.8377154049
O	0.8348554046	-1.9799068325	0.4797069828
C	2.8562230683	-0.0697641436	0.6995070124
O	3.6045656741	-0.7813974348	0.1894201081
O	2.1225781583	0.6624285278	1.2173100971
C	-2.9149823140	0.1929113064	-0.8481651329
O	-3.6263136901	-0.3197045301	-0.0977900268
O	-2.2245556850	0.7220462469	-1.6097114774
C	0.4281555302	1.4590742585	-1.0168780064
O	0.0901127042	2.4881236956	-0.6207050734
O	0.7992758022	0.4404323654	-1.4224592972
H	-0.3454463431	1.8486571894	2.0565623316
C	-0.7615064745	0.8509327985	2.1860759807
H	-1.7471525038	0.8902629428	2.6473897643
H	-0.0820053923	0.2224131111	2.7584608900
F	-0.9073602873	0.2809568642	0.9173937791



C	-2.6643804820	0.0044575644	-0.1365362502
O	-2.8910767126	0.0015721266	-1.2694299146
O	-2.4552750587	0.0073428627	0.9989086285
C	0.0224264025	2.5539908727	-0.2410340436
O	-1.1327766841	2.5444743495	-0.2777693833
O	1.1770607198	2.5758749049	-0.2356473112
C	2.6621855996	-0.0023187275	-0.1987232559
O	2.8950730005	-0.0007450625	-1.3303928771
O	2.4489883945	-0.0040184404	0.9359484082
C	0.0153875839	-2.5557761491	-0.2333520458
O	1.1699548363	-2.5813825076	-0.2300456766
O	-1.1398375805	-2.5426654111	-0.2682018560
C	0.0122692251	0.0042314695	2.1890660775
O	0.0145763656	1.1592764276	2.1919121836
O	0.0097501812	-1.1507927335	2.1927886214
H	-0.6811225548	-0.8977040375	-2.5861283107
C	-0.1170017691	-0.0083403735	-2.3096204968
H	-0.6692386277	0.8856560965	-2.5950946453
H	0.8858239222	-0.0169568904	-2.7302753543
F	0.0119686893	-0.0022172488	-0.9079853536

CH₂F₂-CO₂

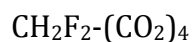
C	1.5219974772	0.1666865452	0.1614904922
O	1.2000540447	1.1906726086	-0.2709424172
O	1.8595506342	-0.8475821525	0.5930231946
H	-1.4333627225	1.1835593646	-0.7236193409
C	-1.6228559381	0.1671380911	-0.3814396664
H	-2.6655860492	-0.1404714791	-0.4486991067
F	-1.2177407401	0.0602017111	0.9105727142
F	-0.8662461366	-0.6879259317	-1.1171877993

CH₂F₂-(CO₂)₂

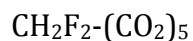
C	-2.1268726337	0.2301564355	0.0057852822
O	-2.0661193938	1.0934997578	-0.7573133580
O	-2.2063819145	-0.6328885121	0.7712700723
C	1.1642733251	1.3357093623	0.1591336535
O	0.4172363882	0.9816937714	0.9713615003
O	1.9067469081	1.7008093790	-0.6415432329
H	0.1001410508	-1.7285887617	0.9335983730
C	0.6488749632	-1.8575312346	0.0020730138
H	0.7114632878	-2.8876565354	-0.3449095324
F	1.9058309276	-1.3679760457	0.1551084753
F	0.0402724516	-1.1109614942	-0.9633901340

CH₂F₂-(CO₂)₃

C	2.3404774752	0.6218330878	0.9291341718
O	1.8555708262	1.6361830394	0.6577313096
O	2.8393403236	-0.3801671832	1.2076595517
C	-1.3298049242	-0.6146863242	1.4618313627
O	-2.4435503753	-0.6928321221	1.7396288938
O	-0.2033384554	-0.5506043813	1.1942658545
C	0.5458554382	-1.3997163651	-1.3640833214
O	-0.1428667770	-2.3217146888	-1.3050710414
O	1.2484579171	-0.4818528376	-1.4340756237
H	-1.5602852677	2.3686309536	-1.5680548477
C	-1.0855080789	1.6665641777	-0.8845415044
H	0.0019669399	1.7009662580	-0.8803654050
F	-1.4797787611	0.4024846773	-1.2233162301
F	-1.5401510884	1.9031509665	0.3727256508



C	-2.6416341430	0.4943748181	0.0926693976
O	-2.5883304060	-0.2935583452	-0.7496500713
O	-2.7118083908	1.2892205493	0.9284707589
C	2.4128849056	-0.0889776196	-0.0428995622
O	2.0445052626	-0.4308671118	0.9997863486
O	2.7860189681	0.2462258392	-1.0808191648
C	-0.1341730733	-0.6653846528	-2.1236452039
O	-0.4768855237	0.0357875309	-2.9699987570
O	0.2201066353	-1.3801959592	-1.2828662361
C	-0.2428718395	-1.9821305942	1.4216113196
O	0.3220443314	-2.9773452106	1.2977770404
O	-0.8266857939	-0.9915192807	1.5688146548
H	0.1036537825	1.3136251355	1.7854931865
C	0.1989399911	1.9938724133	0.9416909744
H	-0.4610124507	2.8579308971	0.9823779877
F	-0.0799981702	1.2926263617	-0.2035409922
F	1.4836862810	2.4139170641	0.8415790792



C	2.7488133786	0.9639895911	0.2958731661
O	2.9883296187	2.0819179749	0.1581626404
O	2.5229816404	-0.1624268360	0.4466866911
C	-2.1854654988	-1.7460629578	-0.3896292164
O	-2.0760516121	-2.8337948628	-0.0254214861
O	-2.3149538186	-0.6600385081	-0.7701086025
C	0.1078738653	0.0029060538	1.9937543504
O	-0.3490261504	-0.9708716319	1.5667484973
O	0.5719570719	0.9632865386	2.4318088494
C	1.0922101872	-2.3966195704	-0.4475447828
O	1.6890257383	-3.0569575841	0.2821901893
O	0.4877759471	-1.7491955302	-1.1955921571
C	-2.3797128537	1.8993830210	0.3008110325
O	-2.2641562425	1.4430747302	1.3555650844
O	-2.5041891796	2.3691134241	-0.7471970465
H	-0.4919173795	0.3393192790	-2.1639370161
C	0.1331445571	1.1553794770	-1.8124253155
H	-0.1581891683	2.1388125788	-2.1764431325
F	1.4239210238	0.9166999624	-2.1495964843
F	0.0788721867	1.1778235710	-0.4409500069

CHF₃-CO₂

C	2.0453625569	0.1277706599	0.1073957274
O	1.5605025353	0.8211569965	0.8974878276
O	2.5340227276	-0.5603879366	-0.6769592912
H	-1.0823122885	0.8306548458	0.9956396227
C	-1.2412067948	0.1151468605	0.1922447140
F	-0.7086725945	0.5640696008	-0.9488254762
F	-2.5380010156	-0.1042684004	-0.0091166343
F	-0.6572466693	-1.0524070496	0.4808157209

CHF₃-(CO₂)₂

C	1.4216350529	1.8658094921	0.1059816986
O	0.6330425269	2.2586095151	-0.6436735697
O	2.2127436004	1.4858597034	0.8541488789
C	1.2268215017	-1.7313394705	-0.4638742346
O	1.1352265500	-0.7033673908	-0.9914959748
O	1.3224612242	-2.7544580710	0.0545973039
H	-1.2479273390	0.6259046741	-0.8843929954
C	-1.5667468423	0.0886045882	0.0056714902
F	-2.7789850116	0.4680668195	0.3967042941
F	-0.7127261633	0.3114236254	1.0150348106
F	-1.5914001807	-1.2310042325	-0.2154935689

CHF₃-(CO₂)₃

C	1.8717314551	0.3513318445	-1.3223366553
O	2.3724185198	1.1655773218	-0.6730913677
O	1.3764859029	-0.4573190090	-1.9809712084
C	0.5054369193	-1.7929616177	1.4930931969
O	1.1761417948	-0.9716196163	1.0226701889
O	-0.1413127724	-2.6095186115	1.9806287717
C	-1.3892910966	-1.0642482487	-1.6471659360
O	-1.1269262969	-1.7126703617	-0.7251816731
O	-1.6667740839	-0.4270607946	-2.5665185823
H	0.7197262375	1.5783996924	1.2605529714
C	-0.3378552712	1.5554056878	1.0090198549
F	-0.8981238305	2.7527751512	1.1412832862
F	-0.9993794316	0.6938142063	1.7863911855
F	-0.5014421903	1.1598201909	-0.2654745050

CHF₃-(CO₂)₄

C	-0.0740673057	2.1152047963	1.1682911660
O	-0.6325515897	1.1664047116	1.5311250265
O	0.4678052578	3.0699980805	0.8217638893
C	-2.9397218041	0.2301118580	0.1819853196
O	-2.5237658585	0.7883750702	-0.7429382775
O	-3.3678328194	-0.3194332497	1.1000004972
C	-0.1019966883	0.2751047034	-2.0987541364
O	0.4600825993	0.8274610402	-1.2476355583
O	-0.6455168628	-0.2717594843	-2.9522239744
C	2.8840948044	0.4603356235	0.0729652260
O	3.4867729734	0.3152366204	-0.8970500963
O	2.2903653800	0.6066155953	1.0576063382
H	0.3842576769	-1.0158029082	1.4508157793
C	0.2468775352	-1.7724298272	0.6829166137
F	-0.8325932697	-1.4932801751	-0.0652891211
F	0.0870658993	-2.9833931330	1.2028825820

CHF₃-(CO₂)₅

C	-0.0385492251	-0.7721177656	1.8484661753
O	0.5456781878	-0.8192361506	0.8454762876
O	-0.5915597525	-0.7327651034	2.8547032307
C	2.8994485560	-2.0425929760	-0.1870684001
O	3.4419273774	-1.0456844145	0.0389439051
O	2.3724107018	-3.0444338367	-0.4050213030
C	0.0918166889	-0.5563486733	-1.8559535689
O	-1.0531534302	-0.4529886138	-1.7410467066
O	1.2346580233	-0.6602424022	-1.9861347925
C	-2.1549326512	1.6595733043	-0.1434709642
O	-2.3860733075	2.3652194930	-1.0227030492
O	-1.9309929553	0.9539731724	0.7488087102
C	-2.9980623561	-1.5495650388	0.0143941073
O	-2.1577258924	-2.1122768569	0.5746958478
O	-3.8429929174	-0.9955876097	-0.5429744327
H	2.2565385724	0.9696363037	-0.0003863615
C	1.6315982168	1.8422233387	0.1739084702
F	0.5409246275	1.8034697120	-0.6170217307
F	2.2805081624	2.9719578485	-0.0866277918
F	1.2041577338	1.8859212742	1.4389865963