

Supplementary Material

Strategies for Red-Shifting Type I Photoinitiators: Internal Electric Fields vs Lewis Acids vs Increasing Conjugation

Nicholas S. Hill and Michelle L. Coote*

ARC Centre of Excellence for Electromaterials Science, Research School of Chemistry,
Australian National University, Canberra ACT 2601, Australia

* Correspondence to michelle.coote@anu.edu.au

Contents

Complexation Thermodynamics Summary	S2
Vertical Excitation Energies	S2
Gaussian Archive Entries	S5

Complexation Thermodynamics Summary

Table S1. MnCl₂ – Gibbs Free Energy (kJ mol⁻¹) of Complexation at Position 1

Mn	Gas	Toluene	DCM	Acetonitrile	H ₂ O
Mg	-145.47	-114.40	-102.72	-85.90	-86.79
Ca	-128.06	-51.71	6.52	33.38	24.22
Zn	-94.15	-52.59	-9.80	8.21	1.69

Table S2. MnCl₂ – Gibbs Free Energy (kJ mol⁻¹) of Complexation at Position 2

Mn	Gas	Toluene	DCM	Acetonitrile	H ₂ O
Mg	-129.99	-93.91	-71.03	-55.47	-59.74
Ca	-116.47	-34.70	34.24	60.63	29.70
Zn	-84.75	-40.73	3.73	20.59	5.79

Table S3. Mn²⁺ – Gibbs Free Energy (kJ mol⁻¹) of Complexation at Position 1

Mn	Gas	Toluene	DCM	Acetonitrile	H ₂ O
Mg	-775.79	-326.03	-155.17	-105.18	-118.60
Ca	-506.79	-117.44	4.92	36.08	13.11
Zn	-921.23	-270.63	-42.69	20.83	-37.45

Table S4. Mn²⁺ – Gibbs Free Energy (kJ mol⁻¹) of Complexation at Position 2

Mn	Gas	Toluene	DCM	Acetonitrile	H ₂ O
Mg	-665.10	-231.41	-95.75	-60.69	-87.81
Ca	-408.59	-53.56	38.79	51.86	23.21
Zn	-847.41	-172.77	13.76	52.64	-22.47

Vertical Excitation Energies

Table S5. Irgacure 2959 Vertical Excitation Energies (eV)

Solvent	S(<i>nπ</i> [*])	S(<i>ππ</i> [*])	T(<i>ππ</i> [*])
Gas	4.0677	5.0482	3.5663
Toluene	4.1029	4.8575	3.5025
DCM	4.1335	4.7993	3.4642
Acetonitrile	4.1416	4.8004	3.4561
H ₂ O	4.158	4.7714	3.4594

Table S6. COOH functionalised Vertical Excitation Energies (eV)

Position	State	Gas	Toluene	DCM	Acetonitrile	H ₂ O
<i>Ortho</i> -	S(<i>nπ</i> [*])	3.9824	4.012	4.0303	4.0378	4.0667
	S(<i>ππ</i> [*])	5.034	4.9041	4.8406	4.8381	4.7812

	$T(\pi\pi^*)$	3.7753	3.7097	3.5692	3.568	3.5238
<i>Meta-</i>	$S(n\pi^*)$	4.0558	4.1018	4.1222	4.1414	4.1397
	$S(\pi\pi^*)$	4.991	4.8578	4.8186	4.8094	4.7634
	$T(\pi\pi^*)$	3.542	3.4958	3.4739	3.458	3.4479
<i>Para-</i>	$S(n\pi^*)$	4.0687	4.1011	4.1345	4.1413	4.1157
	$S(\pi\pi^*)$	5.0268	4.8886	4.8662	4.87	4.8501
	$T(\pi\pi^*)$	3.5499	3.5196	3.5072	3.5019	3.5155

Table S7. COO⁻ functionalised Vertical Excitation Energies (eV)

Position	State	Gas	Toluene	DCM	Acetonitrile	H ₂ O
<i>Ortho-</i>	$S(n\pi^*)$	3.9548	3.9453	3.973	3.9417	4.0105
	$S(\pi\pi^*)$	5.0346	5.029	5.074	5.0874	4.9027
	$T(\pi\pi^*)$	3.9863	3.9905	3.9536	3.964	3.8614
<i>Meta-</i>	$S(n\pi^*)$	4.1447	4.1828	4.1599	4.1597	4.1584
	$S(\pi\pi^*)$	4.2795	4.412	4.5491	4.5894	4.6913
	$T(\pi\pi^*)$	3.3255	3.2075	3.2939	3.3177	3.4004
<i>Para-</i>	$S(n\pi^*)$	4.268	4.2202	4.1917	4.1845	4.1492
	$S(\pi\pi^*)$	3.9966	4.3394	4.5603	4.6093	4.721
	$T(\pi\pi^*)$	3.0044	3.2009	3.3216	3.3471	3.434

Table S8. NMe₂ functionalised Vertical Excitation Energies (eV)

Position	State	Gas	Toluene	DCM	Acetonitrile	H ₂ O
<i>Ortho-</i>	$S(n\pi^*)$	4.1655	4.1983	4.2139	4.2124	4.1014
	$S(\pi\pi^*)$	5.0038	4.9421	4.9041	4.9022	4.7954
	$T(\pi\pi^*)$	3.964	3.9614	3.9499	3.9426	3.8344
<i>Meta-</i>	$S(n\pi^*)$	4.0646	4.0971	4.1273	4.1353	4.1386
	$S(\pi\pi^*)$	4.9196	4.7665	4.7231	4.7471	4.6945
	$T(\pi\pi^*)$	3.4877	3.4415	3.4152	3.424	3.4192
<i>Para-</i>	$S(n\pi^*)$	4.079	4.1162	4.1488	4.1519	4.1446
	$S(\pi\pi^*)$	4.9489	4.8289	4.7797	4.7803	4.7506
	$T(\pi\pi^*)$	3.5036	3.4873	3.4537	3.4482	3.4544

Table S9. NMe₂H⁺ functionalised Vertical Excitation Energies (eV)

Position	State	Gas	Toluene	DCM	Acetonitrile	H ₂ O
<i>Ortho-</i>	$S(n\pi^*)$	4.0904	3.8122	4.1103	4.1024	4.0864
	$S(\pi\pi^*)$	4.6204	4.6967	4.6909	4.7435	4.7467
	$T(\pi\pi^*)$	3.3175	3.5026	3.4714	3.5016	3.5098
<i>Meta-</i>	$S(n\pi^*)$	3.8944	4.0046	4.078	4.1144	4.0951
	$S(\pi\pi^*)$	5.2811	5.0674	4.9306	4.8858	4.8442
	$T(\pi\pi^*)$	3.7454	3.6793	3.5407	3.5133	3.5009
<i>Para-</i>	$S(n\pi^*)$	3.9065	4.0171	4.0934	4.1201	4.1382
	$S(\pi\pi^*)$	5.3932	5.1136	4.9501	4.9043	4.8212

	T($\pi\pi^*$)	3.8137	3.7227	3.574	3.5356	3.4965
--	-----------------	--------	--------	-------	--------	--------

Table S10. I2959-CaCl_n complex Vertical Excitation Energies (eV)

Solvent	S($n\pi^*$)	S($\pi\pi^*$)	T($\pi\pi^*$)
Gas	4.2405	4.6527	3.2697
Toluene	4.2475	4.5698	3.2808
DCM	4.2582	4.6053	3.3157
Acetonitrile	4.2479	4.6263	3.3263
H ₂ O	4.1775	4.6804	3.4074

Table S11. I2959-MgCl_n complex Vertical Excitation Energies (eV)

Solvent	S($n\pi^*$)	S($\pi\pi^*$)	T($\pi\pi^*$)
Gas	4.3762	4.6345	3.2594
Toluene	4.4996	4.4285	3.1776
DCM	4.5885	4.39	3.1129
Acetonitrile	4.6018	4.3905	3.1005
H ₂ O	4.5908	4.4279	3.1597

Table S12. I2959-Zn_n complex Vertical Excitation Energies (eV)

Solvent	S($n\pi^*$)	S($\pi\pi^*$)	T($\pi\pi^*$)
Gas	4.2706	4.6651	3.2833
Toluene	4.4115	4.4734	3.1922
DCM	4.5284	4.4201	3.1745
Acetonitrile	4.5549	4.4065	3.1312
H ₂ O	4.4273	4.5179	3.2438

Table S13. I2959-Ethene Vertical Excitation Energies (eV)

Position	State	Gas	Toluene	DCM	Acetonitrile	H ₂ O
<i>Ortho-</i>	S($n\pi^*$)	3.9123	3.9397	3.9591	3.9652	3.9919
	S($\pi\pi^*$)	4.7302	4.6478	4.6281	4.6408	4.5708
	T($\pi\pi^*$)	3.4163	3.4126	3.4050	3.4082	3.4022
<i>Meta-</i>	S($n\pi^*$)	4.0666	4.1043	4.1398	4.1486	4.1592
	S($\pi\pi^*$)	4.6981	4.6161	4.5676	4.5545	4.5606
	T($\pi\pi^*$)	3.2602	3.3568	3.2241	3.3254	3.255

Table S14. I2959-Butene Vertical Excitation Energies (eV)

Position	State	Gas	Toluene	DCM	Acetonitrile	H ₂ O
<i>Ortho-</i>	S($n\pi^*$)	3.8811	4.127	4.149	4.1656	3.9612
	S($\pi\pi^*$)	4.3404	4.3774	4.3337	4.3506	4.2223
	T($\pi\pi^*$)	2.8379	2.8365	2.7837	2.7774	2.8532

<i>Meta-</i>	$S(n\pi^*)$	4.0637	4.1001	4.1301	4.1339	4.133
	$S(\pi\pi^*)$	4.4231	4.2811	4.2809	4.2369	4.2797
	$T(\pi\pi^*)$	2.8059	2.8101	2.7678	2.7759	2.7699

Table S15. I2959-Hexene Vertical Excitation Energies (eV)

Position	State	Gas	Toluene	DCM	Acetonitrile	H ₂ O
<i>Ortho-</i>	$S(n\pi^*)$	3.8275	4.1325	4.1448	3.9824	4.0088
	$S(\pi\pi^*)$	4.0338	3.8727	3.8617	3.829	3.8092
	$T(\pi\pi^*)$	2.3712	2.352	2.3348	2.3853	2.3866
<i>Meta-</i>	$S(n\pi^*)$	4.0684	4.1039	4.1346	4.1432	4.1292
	$S(\pi\pi^*)$	4.0375	3.8162	3.8064	3.8398	3.8677
	$T(\pi\pi^*)$	2.3341	2.334	2.3245	2.3343	2.3419

Table S16. I2959-Phenyl Vertical Excitation Energies (eV)

Position	State	Gas	Toluene	DCM	Acetonitrile	H ₂ O
<i>Ortho-</i>	$S(n\pi^*)$	3.9017	3.9297	3.9568	3.9736	3.9159
	$S(\pi\pi^*)$	4.8922	4.8287	4.7614	4.7073	4.6786
	$T(\pi\pi^*)$	3.8427	3.8412	3.6988	3.6595	3.7032
<i>Meta-</i>	$S(n\pi^*)$	4.0621	4.0997	4.1322	4.1389	4.1317
	$S(\pi\pi^*)$	4.7691	4.6999	4.6655	4.6649	4.6226
	$T(\pi\pi^*)$	3.4813	3.4482	3.4146	3.4081	3.3954

Table S17. I2959-Phenyl (fused) Vertical Excitation Energies (eV)

State	Gas	Toluene	DCM	Acetonitrile	H ₂ O
$S(n\pi^*)$	3.9037	3.9356	3.9543	3.9636	3.9984
$S(\pi\pi^*)$	4.2518	4.171	4.1575	4.1696	4.1323
$T(\pi\pi^*)$	2.9259	2.9244	2.9161	2.9198	2.9123

Table S18. I2959-Antiaromatic (fused) Vertical Excitation Energies (eV)

State	Gas	Toluene	DCM	Acetonitrile	H ₂ O
$S(n\pi^*)$	3.9158	3.9388	3.9496	3.9522	3.9776
$S(\pi\pi^*)$	2.1933	2.177	2.18	2.1812	2.1872
$T(\pi\pi^*)$	1.4677	1.472	1.4801	1.4821	1.4863

Gaussian Archive Entries

I2959 Gas

```
1\1\GINC-R146\SP\RM062X TD-FC\6-31+G(d,p)\C12H16O4\ROOT\05-Dec-2018\0\
\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50) g
uess=read geom=allcheck maxdisk=2147483648\title\0,1\C,0,-1.18702723
```

04,2.1634135444,-2.7998114936\C,0,0.0283446168,1.3281459892,-2.4538806
379\O,0,-0.0220651449,1.1275059589,-1.0457932803\C,0,0.9234233586,0.35
33064546,-0.4614586327\C,0,1.9740269146,-0.2544156876,-1.1519763358\H,
0,2.0866837618,-0.1335610164,-2.2221491452\C,0,2.8960038165,-1.0313022
74,-0.4522655784\H,0,3.696926418,-1.4885441738,-1.0182636204\C,0,2.793
8991102,-1.2156951888,0.9286150751\C,0,1.7275960053,-0.591653686,1.602
6115305\H,0,1.6454229289,-0.7319360237,2.674984861\C,0,0.805542266,0.1
806769043,0.9250483847\H,0,-0.0165750673,0.6647840489,1.4411344158\C,0
,3.7298645315,-2.0274889443,1.7624027958\C,0,4.9514691704,-2.777369070
6,1.1860259263\C,0,4.5147694616,-3.8656749747,0.1968483071\C,0,5.96460
42348,-1.7984731949,0.5787150583\O,0,5.5997503139,-3.4292393919,2.2568
208755\O,0,-2.3824998322,1.4842620347,-2.4911293402\O,0,3.5363664994,-
2.1157079418,2.9650376252\H,0,-1.1996443224,2.3575920975,-3.8752898564
\H,0,-1.1268482363,3.1263457031,-2.2741900122\H,0,0.955646543,1.847850
1664,-2.7288144958\H,0,-0.0208311198,0.3597100101,-2.9673328889\H,0,4.
082917448,-3.4711532735,-0.7242097625\H,0,3.7857632381,-4.5280977729,0
.6716712992\H,0,5.3985310763,-4.4581765172,-0.054175237\H,0,5.60617803
45,-1.3040505402,-0.325484847\H,0,6.8671798076,-2.365351975,0.33560371
96\H,0,6.231326988,-1.0353184167,1.3150384762\H,0,5.096104936,-3.22959
449,3.0628036293\H,0,-2.3659745267,1.2681646418,-1.5504918154\\Version
=ES64L-G16RevA.03\State=1-A\HF=-767.5142229\RMSD=5.116e-09\PG=C01 [X(C
12H16O4)]\@

I2959 Toluene

1\1\GINC-R82\SP\RM062X TD-FC\6-31+G(d,p)\C12H16O4\ROOT\06-Dec-2018\0\
M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=toluen
e) td(nstates=10,50-50) guess=read geom=allcheck maxdisk=2147483648\\t
itle\\0,1\C,0,-1.2067271983,2.0632250205,-2.9364544428\C,0,0.015656671
2,1.2785457132,-2.5144117389\O,0,-0.0743204499,1.1391900001,-1.0972005
425\C,0,0.8688163654,0.41634308,-0.4516740788\C,0,1.967513403,-0.17966
00821,-1.0809171884\H,0,2.1211388118,-0.0887844565,-2.1493312219\C,0,2
.877712781,-0.8987119971,-0.3164752459\H,0,3.7317280412,-1.3641750216,
-0.7968799986\C,0,2.7294156581,-1.0434756301,1.0687807797\C,0,1.619168
8571,-0.435027356,1.6796145772\H,0,1.4499107707,-0.513410148,2.7455529
354\C,0,0.7016540374,0.2839882495,0.9325763853\H,0,-0.1553777282,0.754
6095295,1.4025901319\C,0,3.7758921284,-1.837230776,1.7763259032\C,0,3.
7841659979,-2.0626567008,3.304861718\C,0,3.9140071264,-0.7356078784,4.
0603338307\C,0,2.5625305665,-2.8780462971,3.7441879713\O,0,4.931817541
6,-2.8294048788,3.6171485743\O,0,-2.400170881,1.3707698419,-2.63291490
92\O,0,4.6850904066,-2.3443489687,1.1339304864\H,0,-1.185630839,2.2045
083077,-4.0202220029\H,0,-1.1902207364,3.0523601704,-2.4586509888\H,0,
0.9341189268,1.8145748155,-2.7853072262\H,0,0.0129896322,0.2870927197,
-2.9837906533\H,0,3.0336306181,-0.0968778104,3.9740007573\H,0,4.785574
4304,-0.1820097561,3.6984366801\C,0,4.0730791971,-0.9666376491,5.11754
15693\H,0,1.6174828304,-2.3454381374,3.62690021\H,0,2.6904672266,-3.13
09135382,4.8006516786\H,0,2.5111559501,-3.8109074176,3.1748163437\H,0,
5.379512352,-3.0240046611,2.7772737609\H,0,-2.4103654955,1.2036707131,
-1.6814650548\\Version=ES64L-G16RevA.03\State=1-A\HF=-767.5320773\RMSD
=2.942e-09\PG=C01 [X(C12H16O4)]\@

I2959 DCM

1\1\GINC-R386\SP\RM062X TD-FC\6-31+G(d,p)\C12H16O4\ROOT\06-Dec-2018\0\
M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=dichl
oromethane) td(nstates=10,50-50) guess=read geom=allcheck maxdisk=2147
483648\\title\\0,1\C,0,-1.192689797,2.078621953,-2.9355949252\C,0,0.02
25466924,1.2851818238,-2.5129777804\O,0,-0.0716913045,1.1363562675,-1.
0946396675\C,0,0.8668782356,0.4089404741,-0.451287486\C,0,1.9731793737
, -0.1759769921,-1.0799496961\H,0,2.1349618507,-0.0699647455,-2.1459852
388\C,0,2.8784203902,-0.9023891418,-0.3165043391\H,0,3.736630884,-1.35
77387929,-0.7995431789\C,0,2.7199909481,-1.0635846112,1.0670647508\C,0
,1.6027981927,-0.4653661844,1.6775369622\H,0,1.4217837946,-0.558059705
9,2.7404930823\C,0,0.6883493303,0.2583594181,0.9307824913\H,0,-0.17554
62875,0.7170555449,1.400856077\C,0,3.7591468802,-1.8636646235,1.773774
9328\C,0,3.7912097015,-2.051716948,3.3067130001\C,0,3.9000548948,-0.71
16577713,4.0391673066\C,0,2.5908779327,-2.8858033913,3.7702097577\O,0,

4.9649206632,-2.7843507765,3.6208014228\O,0,-2.3963954482,1.3879503995
,-2.6501763241\O,0,4.6444331717,-2.4116218709,1.1277840689\H,0,-1.1591
551977,2.2296183462,-4.0174835144\H,0,-1.1795794478,3.062052071,-2.447
3517101\H,0,0.9427321767,1.8199744849,-2.777325478\H,0,0.0199064476,0.
2965522559,-2.9874894114\H,0,2.9944434051,-0.1078349114,3.9697799033\H
,0,4.7411174375,-0.1335672038,3.6443892476\H,0,4.0929754739,-0.9229322
908,5.0951782061\H,0,1.6346563348,-2.3765147042,3.6403888935\H,0,2.724
8584466,-3.1061188456,4.8334760879\H,0,2.5609495153,-3.8329908958,3.22
26790486\H,0,5.3654293351,-3.0566940204,2.7777796672\H,0,-2.4467770264
,1.2594343883,-1.6927171568\\Version=ES64L-G16RevA.03\State=1-A\HF=-76
7.5384041\RMSD=4.127e-09\PG=C01 [X(C12H16O4)]\@

I2959 Acetonitrile

1\1\GINC-R56\SP\RM062X TD-FC\6-31+G(d,p)\C12H16O4\ROOT\06-Dec-2018\0\
M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=aceton
itrile) td(nstates=10,50-50) guess=read geom=allcheck maxdisk=21474836
48\\title\0,1\C,0,-1.193811046,2.0767869153,-2.934562887\C,0,0.025183
6655,1.2884771019,-2.5143846589\O,0,-0.0658034227,1.1434776823,-1.0944
408749\C,0,0.8707359457,0.4137491,-0.4519108532\C,0,1.979640388,-0.167
537932,-1.0801346818\H,0,2.1457576941,-0.055070097,-2.1449626009\C,0,2
.8818555162,-0.8979820032,-0.3168454571\H,0,3.7416368129,-1.3497282886
, -0.800542739\C,0,2.7186426202,-1.0664186302,1.0657069934\C,0,1.599555
2457,-0.4708237288,1.6758067117\H,0,1.4132218477,-0.568557196,2.737359
1433\C,0,0.6876903485,0.2562661498,0.9290100553\H,0,-0.1781453629,0.71
13757079,1.399134898\C,0,3.7539152906,-1.8706699535,1.7722599402\C,0,3
.7897095035,-2.0515238803,3.3060549016\C,0,3.8962606226,-0.7088564382,
4.033184232\C,0,2.5919667539,-2.8860996475,3.7751506463\O,0,4.96734865
28,-2.7803162388,3.6193957877\O,0,-2.3955010169,1.3866303135,-2.633681
6716\O,0,4.633792511,-2.4281204839,1.1259818651\H,0,-1.1677543779,2.21
91331614,-4.0176977693\H,0,-1.1791296945,3.063832595,-2.4539345075\H,0
,0.9425661446,1.8256293755,-2.7829337357\H,0,0.0257809534,0.2982303056
, -2.9853488589\H,0,2.9862991373,-0.1113572902,3.9671738452\H,0,4.73157
70554,-0.1271096522,3.6313761039\H,0,4.0950995296,-0.915621936,5.08904
48338\H,0,1.6349348499,-2.3790201936,3.6431750844\H,0,2.7267209507,-3.
0989214326,4.8399040987\H,0,2.56354273,-3.8364246245,3.2328130639\H,0,
5.3565612588,-3.0648827466,2.7751271539\H,0,-2.4284341077,1.2530029853
, -1.6764490627\\Version=ES64L-G16RevA.03\State=1-A\HF=-767.538626\RMSD
=1.631e-09\PG=C01 [X(C12H16O4)]\@

I2959 Water

1\1\GINC-R64\SP\RM062X TD-FC\6-31+G(d,p)\C12H16O4\ROOT\06-Dec-2018\0\
M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=h2o) t
d(nstates=10,50-50) guess=read geom=allcheck maxdisk=2147483648\\title
\0,1\C,0,-1.2096830393,2.0964705709,-2.8210125531\C,0,0.0223854215,1.
3132889637,-2.4363401884\O,0,-0.0551798301,1.0837394563,-1.0257473442\
C,0,0.9214190519,0.3516731286,-0.4366566856\C,0,2.0290069543,-0.162437
9357,-1.1168593451\H,0,2.1671707247,0.0105975833,-2.176783304\C,0,2.97
49709158,-0.9092868874,-0.4189602671\H,0,3.8216854449,-1.2845778533,-0
.9792269439\C,0,2.8465980745,-1.1444796236,0.9553602036\C,0,1.72676501
74,-0.6074483746,1.6202004413\H,0,1.6082925286,-0.7825569892,2.6840757
874\C,0,0.7731764142,0.123979811,0.940043747\H,0,-0.0949479875,0.52849
91808,1.4501977325\C,0,3.8162837598,-1.912202941,1.7781337022\C,0,4.92
05980733,-2.804332484,1.1744857966\C,0,4.3735044008,-3.8042294022,0.15
83945477\C,0,6.0400725894,-1.9273445101,0.6004031445\O,0,5.4665542603,
-3.5778261768,2.2386711078\O,0,-2.4021164304,1.3450295386,-2.631373527
5\O,0,3.7559693235,-1.8511661981,3.0040739097\H,0,-1.1518207819,2.3384
054871,-3.8845689391\H,0,-1.249547333,3.0322216708,-2.2510279089\H,0,0
.9250615356,1.8880996883,-2.6727907023\H,0,0.047640882,0.3523122633,-2
.9626732311\H,0,4.0495793757,-3.3274110343,-0.7666362436\H,0,3.5324950
035,-4.3587808561,0.5848375632\H,0,5.1727451576,-4.5112057492,-0.08263
93416\H,0,5.7199422548,-1.3331243779,-0.2568822226\H,0,6.8532684062,-2
.5852857272,0.2803635167\H,0,6.4184738565,-1.2525711278,1.3742623552\H
,0,5.270879464,-3.1080117137,3.0668540481\H,0,-2.5143654886,1.18891761
94,-1.6835328556\\Version=ES64L-G16RevA.03\State=1-A\HF=-767.5368437\R
MSD=1.538e-09\PG=C01 [X(C12H16O4)]\@

I2959-COOH Gas

Ortho-

```
1\1\GINC-R1168\SP\RM062X TD-FC\6-31+G(d,p)\C14H18O6\ROOT\09-Jan-2019\0
\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50)
maxdisk=2684354560\title\0,1\C,0,-1.5965369126,1.9649587825,-2.69048
52757\C,0,-1.8847132177,3.0154885606,-3.7429752423\O,0,-2.0112814066,4
.2477737626,-3.0432799088\C,0,-2.3388039728,5.3619267944,-3.7445350244
\C,0,-2.4755137698,6.5356644193,-2.9932573045\H,0,-2.3200062264,6.4729
495267,-1.9203933879\C,0,-2.7905089785,7.7468349575,-3.5919122934\C,0,
-2.8674988057,8.9782347162,-2.7172375279\C,0,-3.0096603936,7.7771478,-
4.9885510136\C,0,-2.8877681985,6.5994301548,-5.721960642\H,0,-3.046035
7694,6.6145229459,-6.7952650858\C,0,-2.5360188438,5.3908488837,-5.1240
135107\H,0,-2.4301237449,4.5013240289,-5.7320472665\C,0,-3.3598823279,
9.0690683699,-5.645525097\C,0,-4.4540252636,9.1761061923,-6.7340260607
\C,0,-3.7818921974,9.1204376977,-8.1139835489\C,0,-5.5679604987,8.1438
802066,-6.601504155\O,0,-5.0670254763,10.4431123273,-6.5661599923\O,0,
-2.6615268038,1.8486427356,-1.7749567032\O,0,-2.8087190766,10.10236875
38,-5.3049571971\H,0,-0.6554509207,2.2116184015,-2.1799144295\H,0,-1.4
826056089,0.9904998156,-3.1721171363\H,0,-2.8253810469,2.7847399946,-4
.258757485\H,0,-1.0666270544,3.0767513363,-4.4728965164\H,0,-3.3011963
441,8.1569712443,-8.3080600119\H,0,-3.0272391832,9.9081542677,-8.19421
59229\H,0,-4.5475494984,9.289216685,-8.8760778435\H,0,-5.2471197859,7.
1496330124,-6.9171635508\H,0,-6.3949371989,8.4620135939,-7.2418248681\
H,0,-5.919772008,8.0858306779,-5.5690983829\H,0,-4.3737131771,11.06211
97126,-6.2893620944\H,0,-2.8039462828,2.7157630484,-1.3754606328\H,0,-
2.8341902706,8.6784080081,-1.6645793349\C,0,-4.0828623891,9.8737223682
,-2.8611375281\H,0,-2.009338603,9.6318928957,-2.891554328\O,0,-5.10881
52222,9.2986048483,-3.5200577002\O,0,-4.1458628181,10.9870033237,-2.40
71348396\H,0,-5.8003167031,9.9722801491,-3.6245451571\Version=ES64L-G
16RevA.03\State=1-A\HF=-995.3263341\RMSD=6.264e-09\PG=C01 [X(C14H18O6)
]\@
```

Meta-

```
1\1\GINC-R1169\SP\RM062X TD-FC\6-31+G(d,p)\C14H18O6\ROOT\09-Jan-2019\0
\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50)
maxdisk=2684354560\title\0,1\C,0,-1.9130100888,1.5322271001,-3.11058
06742\C,0,-1.9649629341,2.9213425753,-3.7166564961\O,0,-2.0787145732,2
.7722757343,-5.1287962301\C,0,-2.4698610278,3.8438089773,-5.863089894\
C,0,-3.1407476363,3.5479823232,-7.0648506955\C,0,-3.5461505431,4.59731
23918,-7.8700858736\C,0,-3.4139745292,2.1076441991,-7.4226962703\C,0,-
3.3087506634,5.938244901,-7.5209922649\C,0,-2.6572529923,6.2027641558,
-6.314078452\H,0,-2.4578709909,7.217113201,-5.9951320973\C,0,-2.241496
5247,5.1645742243,-5.4836742863\H,0,-1.734629861,5.3895715688,-4.55246
66581\C,0,-3.7978831612,6.9727311334,-8.4825295305\C,0,-3.6528246343,8
.4919023337,-8.243807398\C,0,-4.4252349792,8.9328312416,-6.9940173559\
C,0,-2.1752733568,8.9032477484,-8.2019651794\O,0,-4.2356820126,9.15720
27225,-9.3435900007\O,0,-3.120189323,0.823270231,-3.2958800706\O,0,-4.
3428042761,6.6181409501,-9.5161767175\H,0,-1.7470352712,1.6353892853,-
2.0331035327\H,0,-1.0632479105,0.9836221704,-3.5346701951\H,0,-1.05052
70848,3.4741457175,-3.4634796576\H,0,-2.8400141449,3.4671607645,-3.341
5036527\H,0,-3.9989313767,8.5577393827,-6.0624185055\H,0,-5.4650823836
,8.6018990709,-7.0635157447\H,0,-4.4179565966,10.0257229276,-6.9699136
579\H,0,-1.6390926881,8.5194314302,-7.3326576105\H,0,-2.1366483327,9.9
956344747,-8.1854144302\H,0,-1.668557029,8.5596309614,-9.1079844628\H,
0,-4.5589379426,8.4756409296,-9.955091569\H,0,-3.0570371389,0.28751020
12,-4.1013956084\H,0,-4.1727771038,2.0641759234,-8.2108691182\C,0,-3.9
042264603,1.2884652098,-6.2482224699\H,0,-2.5175214986,1.6020433577,-7
.7910352327\O,0,-4.8023548797,1.9359855191,-5.4991263521\O,0,-3.533616
1124,0.1593082621,-6.0058019279\H,0,-4.9441793739,1.4233686355,-4.6847
191013\H,0,-4.0768285639,4.3983830637,-8.7963380259\Version=ES64L-G16
RevA.03\State=1-A\HF=-995.3360204\RMSD=8.483e-09\PG=C01 [X(C14H18O6)]\
\@
```

Para-

```
1\1\GINC-R769\SP\RM062X TD-FC\6-31+G(d,p)\C12H14O5\ROOT\16-Apr-2019\0\
```



```
\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50) g
uess=read geom=allcheck maxdisk=2147483648\\title\\0,1\C,-1.1648992393
,2.3114894623,-2.6214616379\C,-0.0596030129,1.2709052852,-2.5389764467
\O,0.5072997856,1.0057445291,-3.7902184178\C,-0.2077728526,0.279469113
8,-4.692030001\C,0.4321002363,0.043039186,-5.9118719429\H,1.4222490778
,0.457087354,-6.0660570208\C,-0.1982545537,-0.7034828175,-6.8933984334
\H,0.328623819,-0.8641977572,-7.8245845314\C,-1.480422793,-1.235658265
5,-6.6830052119\C,-2.1033753311,-0.9844897457,-5.4549020018\H,-3.09667
70649,-1.3884202792,-5.2914510781\C,-1.4867242765,-0.2341913193,-4.462
0919448\H,-2.0158092067,-0.0525571288,-3.5338186377\C,-2.2496633382,-2
.0543768131,-7.6674561207\C,-1.7235161781,-2.4011184012,-9.0775894313\
C,-1.5111936784,-1.1343746258,-9.9159229118\C,-0.4644467959,-3.2741058
966,-8.9943678107\O,-2.7142741711,-3.1660073256,-9.7301306227\O,-1.729
0954421,2.4855182411,-1.4122289799\O,-3.3526658752,-2.4810119881,-7.36
18474392\O,-1.4922934572,2.9084561449,-3.6100739386\H,-0.4423242245,0.
3660056373,-2.0512862537\H,0.7403035829,1.6754327191,-1.9137449293\H,-
0.694603548,-0.5056589493,-9.5579923885\H,-2.4299557934,-0.5417390419,
-9.9325034147\H,-1.2913032128,-1.4483959143,-10.9397362911\H,0.4030625
876,-2.7525556513,-8.5872655268\H,-0.2287721079,-3.612018546,-10.00699
86225\H,-0.6649580064,-4.1564430007,-8.3802915493\H,-3.4499504112,-3.2
755298168,-9.1056861389\H,-2.409995518,3.1713626112,-1.496701324\\Vers
ion=ES64L-G16RevA.03\State=1-A\HF=-841.5338486\RMSD=3.410e-09\PG=C01 [
X(C12H14O5)]\\@
```

I2959-COOH Toluene

Ortho-

```
1\1\GINC-R1177\SP\RM062X TD-FC\6-31+G(d,p)\C14H18O6\ROOT\09-Jan-2019\0
\\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=tolu
ene) td(nstates=10,50-50) maxdisk=2684354560\\title\\0,1\C,0,-1.582814
1054,1.9742165578,-2.7210013364\C,0,-1.9048275144,3.0236100637,-3.7617
734203\O,0,-1.9991940499,4.2615620799,-3.0606179104\C,0,-2.3482689915,
5.3726600373,-3.750800236\C,0,-2.4604617409,6.5484188179,-2.9978033081
\H,0,-2.2744345418,6.4893085922,-1.929427798\C,0,-2.7923026701,7.76003
48114,-3.5868578639\C,0,-2.8455978125,8.9816300584,-2.696529755\C,0,-3
.0534483125,7.7929995592,-4.9788319779\C,0,-2.9573721621,6.6091911529,
-5.7109450783\H,0,-3.1473519065,6.6159296009,-6.777940723\C,0,-2.59105
54483,5.4007858926,-5.1234629155\H,0,-2.507493625,4.51085726,-5.734930
1178\C,0,-3.4130519864,9.0833414415,-5.6314489116\C,0,-4.4350706823,9.
1805701068,-6.7899418056\C,0,-3.6960909129,9.0334815797,-8.1283364114\
C,0,-5.5965733338,8.2013677137,-6.6621444061\O,0,-5.0021398683,10.4789
636937,-6.7263440121\O,0,-2.6133299133,1.8596610664,-1.7613160023\O,0,
-2.9184627693,10.1296321672,-5.2392168181\H,0,-0.6221263786,2.21309948
7,-2.2444325575\H,0,-1.4912424428,1.0006011714,-3.2095238793\H,0,-2.86
38643335,2.7985942906,-4.2446134883\H,0,-1.119666003,3.0758128868,-4.
5190262696\H,0,-3.2504352188,8.0449045363,-8.2665741334\H,0,-2.9039529
466,9.7848644983,-8.2037433113\H,0,-4.4144322969,9.2063360475,-8.93505
83227\H,0,-5.3008767998,7.1740557122,-6.8815893322\H,0,-6.3684541011,8
.4991584867,-7.3775894094\H,0,-6.0213643882,8.2354828028,-5.6553491373
\H,0,-4.3243261449,11.0680007877,-6.3590993319\H,0,-2.7304373794,2.725
5257902,-1.3492154438\H,0,-2.773799819,8.6647593797,-1.6501799905\C,0,
-4.0769708366,9.8574496113,-2.7749818827\H,0,-1.999256883,9.6449967842
,-2.8882734469\O,0,-5.135310131,9.2627266043,-3.354588145\O,0,-4.13252
08934,10.9728834222,-2.3177223868\H,0,-5.8617460588,9.9084704477,-3.36
97527235\\Version=ES64L-G16RevA.03\State=1-A\HF=-995.3485251\RMSD=8.45
5e-09\PG=C01 [X(C14H18O6)]\\@
```

Meta-

```
1\1\GINC-R1222\SP\RM062X TD-FC\6-31+G(d,p)\C14H18O6\ROOT\09-Jan-2019\0
\\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=tolu
ene) td(nstates=10,50-50) maxdisk=2684354560\\title\\0,1\C,0,-0.837198
1902,1.7804360739,-2.728322543\C,0,0.4326762863,1.0169088024,-2.414541
7487\O,0,0.5770931363,1.0330933214,-0.9957618189\C,0,1.5389577975,0.28
24432278,-0.4160857185\C,0,1.3997274458,0.1153648761,0.9763707441\C,0,
2.3483238182,-0.6271665673,1.653253254\C,0,0.2147141487,0.7473768335,1
```

.6631943675\C,0,3.4434198489,-1.2121914445,0.9897801264\C,0,3.5481008356,-1.0415614971,-0.3931057079\H,0,4.3646292274,-1.4790742486,-0.9519193681\C,0,2.6018463282,-0.30299271,-1.1008799213\H,0,2.7032981876,-0.1862681055,-2.1733984261\C,0,4.4041402967,-1.9809492849,1.8330399837\C,0,5.6725738435,-2.663162922,1.2721282442\C,0,5.3116895472,-3.7768383173,0.2821101169\C,0,6.6353627506,-1.6306027888,0.6752754729\O,0,6.3420957295,-3.2751186447,2.3583137528\O,0,-1.9809522423,1.155082078,-2.1893049222\O,0,4.2005263739,-2.0844265762,3.0346086678\H,0,-0.9617777918,1.8119551202,-3.8151171317\H,0,-0.7403969451,2.812866767,-2.3672448541\H,0,1.296570686,1.4993701207,-2.8896130416\H,0,0.3524445857,-0.0218499474,-2.7582511681\H,0,4.8897608117,-3.4092717502,-0.6545697252\H,0,4.5996730049,-4.4704636113,0.7392818242\H,0,6.2276176953,-4.3301335936,0.0556819926\H,0,6.258816749,-1.1582675197,-0.2333850968\H,0,7.5717633475,-2.1438006169,0.4382519072\H,0,6.8518538183,-0.8507301276,1.4114790537\H,0,5.8099041697,-3.1039285512,3.1527292976\H,0,-2.040955104,1.3636495069,-1.2449445382\H,0,0.1425170595,0.3751992701,2.6905188965\C,0,-1.0964889936,0.448322364,0.9716960102\H,0,0.3035618637,1.8361244548,1.70086786\O,0,-1.2205609478,-0.8380383456,0.6302083666\O,0,-1.9703709239,1.2635889735,0.7605795207\H,0,-2.0769913217,-0.9537797402,0.1851272235\H,0,2.2536790673,-0.7756128797,2.7246700472\Version=ES64L-G16RevA.03\State=1-A\HF=-995.3572335\RMSD=6.194e-09\PG=C01 [X(C14H18O6)]\@

Para-

1\1\GINC-R770\SP\RM062X TD-FC\6-31+G(d,p)\C12H14O5\ROOT\16-Apr-2019\O\
 \# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50) s
 crf(smd,solvent=toluene) guess=read geom=allcheck maxdisk=2147483648\
 title\0,1\C,-1.1599501356,2.3174470901,-2.6189420542\C,-0.0664749858,
 1.2669558385,-2.5358510973\O,0.5015898979,1.0014948362,-3.7890335923\C
 ,-0.2103398316,0.2756000812,-4.6899729924\C,0.4293058367,0.040226867,-
 5.9110787594\H,1.4200685292,0.452742085,-6.0682873059\C,-0.2004743343,
 -0.7049662492,-6.8939120645\H,0.3293670219,-0.8617817186,-7.8243117115
 \C,-1.483524535,-1.2375800664,-6.6840278179\C,-2.1060629417,-0.9870158
 964,-5.4545310902\H,-3.0994729297,-1.3883582355,-5.2855517724\C,-1.489
 8828813,-0.2386071066,-4.460240994\H,-2.0178513289,-0.0621696043,-3.53
 01301443\C,-2.2498854001,-2.0543917113,-7.6699104028\C,-1.7196427447,-
 2.40513075,-9.0781352091\C,-1.5185326104,-1.1394753558,-9.918899156\C,
 -0.4556008638,-3.267956512,-8.9944581211\O,-2.7088817245,-3.1834666696
 ,-9.7249631906\O,-1.7333808656,2.4901857136,-1.4187167645\O,-3.3582045
 204,-2.4768548804,-7.3708787245\O,-1.4670515463,2.929499347,-3.6077451
 256\H,-0.4533453874,0.3623864234,-2.0514398981\H,0.7357366139,1.664800
 7729,-1.9087282556\H,-0.7098697746,-0.5020264748,-9.5579632017\H,-2.44
 23496343,-0.5537498889,-9.9405963617\H,-1.2875204007,-1.4494345951,-10
 .9421136984\H,0.4109063599,-2.736271402,-8.5987866391\H,-0.219060132,-
 3.61298256,-10.0051226473\H,-0.6423222677,-4.1468760347,-8.3701397832\
 H,-3.4503408388,-3.2717063359,-9.103564714\H,-2.4058626443,3.187639992
 7,-1.4976577104\Version=ES64L-G16RevA.03\State=1-A\HF=-841.5533895\R
 SD=3.151e-09\PG=C01 [X(C12H14O5)]\@

I2959-COOH DCM

Ortho-

1\1\GINC-R988\SP\RM062X TD-FC\6-31+G(d,p)\C14H18O6\ROOT\09-Jan-2019\O\
 \# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=dichl
 oromethane) td(nstates=10,50-50) maxdisk=2684354560\title\0,1\C,0,-1
 .5926929138,1.974200806,-2.731793169\C,0,-1.9064916282,3.029941258,-3.
 7668309681\O,0,-1.98969953,4.2702873631,-3.0630797059\C,0,-2.341131649
 9,5.3807297643,-3.7502108096\C,0,-2.4544005146,6.5561783635,-2.9950012
 041\H,0,-2.267661597,6.4989857787,-1.9263163964\C,0,-2.791422186,7.767
 4043399,-3.5828745347\C,0,-2.8491452712,8.985071943,-2.6866723949\C,0,
 -3.057739867,7.8017487023,-4.9752445512\C,0,-2.9582177909,6.6173079573
 ,-5.709030841\H,0,-3.1477091696,6.6206386344,-6.7757793983\C,0,-2.5865
 866891,5.4098426251,-5.1232530829\H,0,-2.5008997971,4.5210559459,-5.73
 63636792\C,0,-3.4252777294,9.0898490978,-5.6257913656\C,0,-4.426021578
 2,9.1827777258,-6.8036122877\C,0,-3.6693972553,9.0241673006,-8.1301928
 445\C,0,-5.5943294074,8.2106687646,-6.6844234848\O,0,-4.9900746338,10.

485969313,-6.7594744304\O,0,-2.6321156478,1.8497446132,-1.7768928352\O,0,-2.9539081191,10.1422256528,-5.2160896131\H,0,-0.6371770931,2.2074970257,-2.2436782308\H,0,-1.4984710155,1.0059271861,-3.2297067548\H,0,-2.8668194184,2.816705781,-4.2514327786\H,0,-1.1136699952,3.0766883153,-4.5234729318\H,0,-3.2310556779,8.0314412234,-8.2569673365\H,0,-2.8708688531,9.7699350201,-8.1977664783\H,0,-4.3771630628,9.1971223285,-8.9465408865\H,0,-5.2948424006,7.1792254601,-6.8769829161\H,0,-6.3472634913,8.4946174663,-7.4256287503\H,0,-6.0444239708,8.2676928743,-5.6891542847\H,0,-4.3129593662,11.081243694,-6.3990168404\H,0,-2.717662636,2.6963503489,-1.3164089129\H,0,-2.7776210792,8.6616363171,-1.6421107023\C,0,-4.0896372096,9.8448226126,-2.7602863452\H,0,-2.0059409613,9.6535267748,-2.8736786843\O,0,-5.1513813673,9.2235059924,-3.2960157984\O,0,-4.1485018089,10.9741382515,-2.3296560344\H,0,-5.9020436173,9.8450723785,-3.2935517371\\Version=ES64L-G16RevA.03\State=1-A\HF=-995.3577708\RMSD=7.370e-09\PG=C01 [X(C14H18O6)]\@

Meta-

1\1\GINC-R1167\SP\RM062X TD-FC\6-31+G(d,p)\C14H18O6\ROOT\09-Jan-2019\O\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=dichloromethane) td(nstates=10,50-50) maxdisk=2684354560\title\0,1\C,0,-0.8361348707,1.786569086,-2.7420669763\C,0,0.4467719125,1.0505107662,-2.4221478941\O,0,0.5460593259,1.018025034,-0.996939125\C,0,1.5392139781,0.3137367525,-0.4138519534\C,0,1.3962630086,0.1337839483,0.9773524518\C,0,2.3715102216,-0.5689209723,1.6594055944\C,0,0.1816638362,0.7138172062,1.6580204405\C,0,3.4928936051,-1.1087950157,0.999885027\C,0,3.6034482146,-0.9235454351,-0.3817745734\H,0,4.4466230268,-1.3122386368,-0.9375667438\C,0,2.6356496215,-0.2159993406,-1.0926268409\H,0,2.7465675193,-0.0808335837,-2.1621535781\C,0,4.4768126165,-1.8413719481,1.8458076129\C,0,5.6379571304,-2.6827636874,1.2696739427\C,0,5.1445103141,-3.7523599597,0.2939269891\C,0,6.7025525426,-1.7671759403,0.6511945701\O,0,6.2397114162,-3.3716624247,2.3543347745\O,0,-1.9762766667,1.11272269,-2.2431650203\O,0,4.3771491091,-1.7918035125,3.0655236711\H,0,-0.9411861757,1.8446972892,-3.8291109139\H,0,-0.7799328715,2.8093637869,-2.3472561828\H,0,1.3075271957,1.5780666144,-2.8503200033\H,0,0.4135243325,0.023359119,-2.8048842201\H,0,4.7805423796,-3.3376257819,-0.6469898962\H,0,4.3457437917,-4.3435508681,0.751911993\H,0,5.9843613373,-4.4184108592,0.074927865\H,0,6.3563401991,-1.2444588633,-0.2423298944\H,0,7.5611257009,-2.3879071405,0.3782002407\H,0,7.0318416873,-1.0259421205,1.3861413022\H,0,5.8858565502,-2.9826434859,3.1717516609\H,0,-2.0179465477,1.2351429336,-1.282433239\H,0,0.129924474,0.3537028938,2.6909531147\C,0,-1.1112380564,0.333695545,0.9750135977\H,0,0.2166104455,1.8060796729,1.676802559\O,0,-1.1775871918,-0.9661674392,0.6749818869\O,0,-2.0212967049,1.1025990277,0.7335142085\H,0,-2.036144164,-1.1447996253,0.2492252905\H,0,2.2706337566,-0.7213437248,2.729789262\\Version=ES64L-G16RevA.03\State=1-A\HF=-995.3651405\RMSD=5.673e-09\PG=C01 [X(C14H18O6)]\@

Para-

1\1\GINC-R52\SP\RM062X TD-FC\6-31+G(d,p)\C12H14O5\ROOT\16-Apr-2019\O\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50) scrf(smd,solvent=dichloromethane) guess=read geom=allcheck maxdisk=2147483648\title\0,1\C,-1.200051732,2.2776370904,-2.6781292349\C,-0.1128958762,1.2314343924,-2.521163516\O,0.5753904896,1.0127223425,-3.7266895447\C,-0.0358694555,0.3199856897,-4.7214435527\C,-1.3172156612,-0.2287904687,-4.6352624711\H,-1.9292140656,-0.1157594657,-3.7476691528\C,-1.8327268704,-0.936721007,-5.7187859111\H,-2.8283548868,-1.3466191182,-5.613120074\C,-1.0955129275,-1.1072072513,-6.8959946098\C,0.1921705175,-0.5414387796,-6.9582998638\H,0.774718771,-0.6637674512,-7.8651224563\C,0.7189667598,0.1610300316,-5.8919545487\H,1.7111949377,0.5980932985,-5.9387836169\C,-1.5664075593,-1.8432269632,-8.1027973821\C,-2.9550891951,-2.512531623,-8.2073346423\C,-3.1019026477,-3.6426538344,-7.1829207533\C,-4.0787511036,-1.4755453334,-8.1090398663\O,-3.0451841633,-3.1031123218,-9.4943164244\O,-1.8661077058,2.4386191067,-1.5295834593\O,-0.8298948081,-1.9355150389,-9.0772876616\O,-1.4291846241,2.8984636818,-3.6863460877\H,-0.5339755187,0.3092520811,-2.1044217451\H,0.6233178911

,1.6164811573,-1.8103853053\H,-3.144941447,-3.2894775333,-6.1517197653
\H,-2.2690536093,-4.3460580195,-7.2789176641\H,-4.0307929557,-4.176528
7526,-7.4045018324\H,-4.1684364513,-1.0271694651,-7.118614689\H,-5.020
2012102,-1.9797641182,-8.3466990334\H,-3.919822971,-0.6789496267,-8.84
23240953\H,-2.2040974284,-2.9262866814,-9.9491640086\H,-2.5331884929,3
.1403879815,-1.6442540317\\Version=ES64L-G16RevA.03\State=1-A\HF=-841.
5609971\RMSD=2.948e-09\PG=C01 [X(C12H14O5)]\@

I2959-COOH Acetonitrile

Ortho-

1\1\GINC-R3514\SP\RM062X TD-FC\6-31+G(d,p)\C14H18O6\ROOT\09-Jan-2019\0
\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=acet
onitrile) td(nstates=10,50-50) maxdisk=2684354560\\title\0,1\C,0,-1.5
818132187,1.9766996595,-2.7283090497\C,0,-1.9047539754,3.0297148336,-3
.7625183165\O,0,-2.0034424957,4.2686130015,-3.0559679115\C,0,-2.351634
4529,5.3783784673,-3.7450227319\C,0,-2.4655999374,6.5550483279,-2.9912
32725\H,0,-2.2825819504,6.5002605653,-1.9217303074\C,0,-2.7978702273,7
.7663018912,-3.5821031298\C,0,-2.8551411637,8.9846610078,-2.6866701864
\C,0,-3.0600541542,7.7994312937,-4.9754362481\C,0,-2.9614838044,6.6134
279996,-5.707688271\H,0,-3.1472242959,6.6145226705,-6.775136742\C,0,-2
.5936014411,5.4061264002,-5.1190065092\H,0,-2.507646607,4.5166011028,-
5.7311040709\C,0,-3.4201621426,9.0878616664,-5.6290680546\C,0,-4.42173
97303,9.1844697534,-6.8057944413\C,0,-3.6685346936,9.0184866789,-8.133
0151302\C,0,-5.5944798526,8.2187184657,-6.6833591069\O,0,-4.977475439,
10.4922805764,-6.7626456344\O,0,-2.6206513054,1.8428643881,-1.77223581
46\O,0,-2.9408953207,10.13849759,-5.222827055\H,0,-0.6288671617,2.2184
278538,-2.2395130071\H,0,-1.4789507883,1.0099395005,-3.2271325952\H,0,
-2.8610422836,2.8077886728,-4.2508409402\H,0,-1.110594147,3.0863620719
, -4.5167327191\H,0,-3.2358268671,8.0231197274,-8.2569903018\H,0,-2.866
5214766,9.760220706,-8.2045812691\H,0,-4.3775714088,9.1915835494,-8.94
83078245\H,0,-5.296944166,7.1853332985,-6.868620975\H,0,-6.3438623049,
8.4993149688,-7.4295106092\H,0,-6.047857852,8.2849082283,-5.6900355819
\H,0,-4.2925224772,11.0820605479,-6.408157925\H,0,-2.7234264098,2.6936
16843,-1.3243989021\H,0,-2.7920293975,8.6603966879,-1.6417577821\C,0,-
4.0918085371,9.8481366721,-2.7674302411\H,0,-2.0072314582,9.648609451,
-2.8678481057\O,0,-5.1558343187,9.2247682219,-3.2957308073\O,0,-4.1479
136216,10.9819770138,-2.346936929\H,0,-5.9068351155,9.8464146453,-3.29
55860483\\Version=ES64L-G16RevA.03\State=1-A\HF=-995.3591082\RMSD=7.28
3e-09\PG=C01 [X(C14H18O6)]\@

Meta-

1\1\GINC-R291\SP\RM062X TD-FC\6-31+G(d,p)\C14H18O6\ROOT\09-Jan-2019\0\
\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=aceto
nitrile) td(nstates=10,50-50) maxdisk=2684354560\\title\0,1\C,0,-0.41
97234395,1.4601657688,-2.8361923431\C,0,-0.1158019791,0.8863924889,-0.1
469875544\O,0,1.1277418212,0.1919548421,-1.5989180085\C,0,1.7001910309
, -0.3629724508,-0.510535244\C,0,3.0142130931,-0.8340028812,-0.71317761
14\C,0,3.6785191616,-1.4245783314,0.3448580953\C,0,3.6346021561,-0.670
7630298,-2.0781230152\C,0,3.0732993756,-1.5737026464,1.6084943934\C,0,
1.7723449579,-1.0900682214,1.7827179992\H,0,1.2633640945,-1.1668474847
, 2.7344449032\C,0,1.0843616014,-0.4804512215,0.7349329973\H,0,0.078852
2499,-0.1101889688,0.8970959427\C,0,3.8869866161,-2.2347402516,2.66641
14772\C,0,3.3356764496,-2.596750909,4.0635066583\C,0,3.033910171,-1.32
91688651,4.8717760765\C,0,2.1314017209,-3.5364079224,3.9675728543\O,0,
4.3568331654,-3.3059172294,4.7494620722\O,0,0.5674831838,2.3832977775,
-3.2596286295\O,0,5.0562628989,-2.521922022,2.4380354585\H,0,-1.369401
1085,1.9994326015,-2.7838153615\H,0,-0.5280896706,0.6422293507,-3.5605
079682\H,0,-0.9070364531,0.1930717645,-1.1614445877\H,0,-0.0092025183,
1.6824727186,-0.7233986219\H,0,2.1924147709,-0.7563679324,4.4790973423
\H,0,3.9171580029,-0.6833304588,4.9001358783\H,0,2.7954755283,-1.63439
36814,5.8950422877\H,0,1.2437373795,-3.0545397443,3.5559248429\H,0,1.8
966572122,-3.884884303,4.9778448231\H,0,2.379777928,-4.4055197044,3.35
06310175\H,0,5.1525950005,-3.2662776178,4.1921619842\H,0,1.3777462811,
1.8961694966,-3.4741576845\H,0,4.6939189188,-0.945444869,-2.0376865608

\C,0,3.5480806885,0.7460366868,-2.5945933585\H,0,3.1429303787,-1.30638
4109,-2.8189472341\O,0,3.9085169855,1.6532634847,-1.6826295238\O,0,3.2
132949772,1.057216621,-3.7213044672\H,0,3.8476443353,2.540350705,-2.08
26806213\H,0,4.6932570338,-1.7839564512,0.2028242811\\Version=ES64L-G1
6RevA.03\State=1-A\HF=-995.3664789\RMSD=5.559e-09\PG=C01 [X(C14H18O6)]
\\@

Para-

1\1\GINC-R47\SP\RM062X TD-FC\6-31+G(d,p)\C12H14O5\ROOT\16-Apr-2019\0\
M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50) sc
rf(smd,solvent=acetonitrile) guess=read geom=allcheck maxdisk=21474836
48\\title\\0,1\C,-1.1902015349,2.2733049694,-2.6904393996\C,-0.1125991
78,1.2206491598,-2.5146772388\O,0.5859055528,0.9897262728,-3.713591862
2\C,-0.029090499,0.3076499047,-4.7128440217\C,-1.3175904285,-0.2262063
799,-4.6333249257\H,-1.9314032746,-0.1118902407,-3.7471178928\C,-1.838
5034598,-0.9231722553,-5.7214065086\H,-2.8400646453,-1.3193286253,-5.6
189731562\C,-1.1004550635,-1.0958033814,-6.8982344566\C,0.1944391278,-
0.545626758,-6.9538771739\H,0.7794506886,-0.6701361681,-7.8588389273\C
,0.7275502618,0.144085845,-5.8820427071\H,1.7264620301,0.566452777,-5.
9247236412\C,-1.5785277075,-1.8166294292,-8.1109975317\C,-2.9541701024
,-2.5136742628,-8.2032030991\C,-3.0830635238,-3.6343679948,-7.16750461
92\C,-4.0924000467,-1.4913663833,-8.1118492785\O,-3.0346546633,-3.1217
953302,-9.4837556319\O,-1.8886852235,2.4265711284,-1.5612460481\O,-0.8
591250237,-1.8722894979,-9.101595447\O,-1.3867087123,2.9069626841,-3.6
985564457\H,-0.5430223844,0.3037160242,-2.0968825699\H,0.6192615294,1.
6064163018,-1.799766697\H,-3.1429889157,-3.2676636379,-6.1420658545\H,
-2.2340401983,-4.3202262713,-7.2478092882\H,-3.999199158,-4.190240534,
-7.3883798469\H,-4.1800401684,-1.0294682441,-7.1274733331\H,-5.0286113
811,-2.0128428286,-8.33257064\H,-3.9505563559,-0.7038680927,-8.8585676
062\H,-2.2214773419,-2.8849147644,-9.961396432\H,-2.5490041997,3.13296
0013,-1.6893347194\\Version=ES64L-G16RevA.03\State=1-A\HF=-841.56253\R
MSD=3.510e-09\PG=C01 [X(C12H14O5)]\\@

I2959-COOH Water

Ortho-

1\1\GINC-R1171\SP\RM062X TD-FC\6-31+G(d,p)\C14H18O6\ROOT\09-Jan-2019\0\
\\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=h2o)
td(nstates=10,50-50) maxdisk=2684354560\\title\\0,1\C,0,-1.5256501888
,1.643283902,-2.7717906188\C,0,-0.5805956293,0.6757864508,-2.101253641
5\O,0,-0.1489236935,1.2905111536,-0.8828897484\C,0,0.7023744768,0.6005
674793,-0.0844927482\C,0,1.0848657723,1.2423767326,1.1004266783\H,0,0.
6764334397,2.2262809524,1.3124637062\C,0,1.9676030828,0.6482103295,1.9
898921168\C,0,2.3148682273,1.4078165536,3.2486126265\C,0,2.4690407417,
-0.6478755128,1.7048916887\C,0,2.0579809361,-1.2803123124,0.5259537406
\H,0,-2.4323673818,-2.2637860755,0.2713283966\C,0,1.195029214,-0.671447
9116,-0.3794264407\H,0,0.9216523032,-1.1910651105,-1.2891577735\C,0,3.
442538043,-1.2826421943,2.6305580275\C,0,3.5582974944,-2.8141779818,2.
8169329021\C,0,2.2077234172,-3.5185312291,2.8584938225\C,0,4.496795206
7,-3.3914545106,1.7501766604\O,0,4.1481334973,-3.0298256462,4.09641133
29\O,0,-2.7150414911,1.8408871737,-2.0170980726\O,0,4.1961913176,-0.58
43099802,3.3018006645\H,0,-1.8263316628,1.2263565379,-3.7354888765\H,0
, -1.0181794159,2.5992011065,-2.9471879098\H,0,0.2829403895,0.482095580
3,-2.7477804053\H,0,-1.0909097662,-0.2673930177,-1.8748111251\H,0,1.72
84561703,-3.5494051712,1.8796515691\H,0,1.5368089805,-3.0229602918,3.5
663997303\H,0,2.3715822846,-4.5474592714,3.1913510002\H,0,4.1088689225
, -3.2848553302,0.7355251673\H,0,4.6317624297,-4.4567505199,1.958778506
\H,0,5.4703885684,-2.8947509081,1.8062693681\H,0,4.815958018,-2.337928
6543,4.2304874053\H,0,-2.4808738291,2.2896690109,-1.1929741262\H,0,1.6
152228369,2.2430164392,3.3670086455\C,0,3.6915887978,2.0203719062,3.27
15854435\H,0,2.2331607132,0.783382442,4.1407079397\O,0,4.2045784842,2.
2443618437,2.0571178174\O,0,4.2674887506,2.3465155986,4.2936833248\H,0
,5.0711407784,2.6774274367,2.1530032058\\Version=ES64L-G16RevA.03\Stat
e=1-A\HF=-995.3614607\RMSD=4.619e-09\PG=C01 [X(C14H18O6)]\\@

Meta-

```
1\1\GINC-R1173\SP\RM062X TD-FC\6-31+G(d,p)\C14H18O6\ROOT\09-Jan-2019\0
\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=h2o)
td(nstates=10,50-50) maxdisk=2684354560\title\0,1\C,0,-1.2178139746
,1.0607696794,-2.2641803764\C,0,0.1739218255,0.5173817061,-2.039383615
5\O,0,0.4166955097,0.590354135,-0.6306074398\C,0,1.5260027822,0.007673
514,-0.1210608896\C,0,1.5355625195,-0.1179634089,1.2828432099\C,0,2.63
41389373,-0.6967900049,1.8900275596\C,0,0.3467503208,0.3840147753,2.06
18640078\C,0,3.7304377748,-1.1649224697,1.1399591647\C,0,3.6891636566,
-1.0363506113,-0.2527953174\H,0,4.5087644288,-1.3685616559,-0.87644652
34\C,0,2.5961956198,-0.4509487437,-0.8876301543\H,0,2.5920524295,-0.35
15968485,-1.9665658992\C,0,4.8611701907,-1.7569143714,1.9022325196\C,0
,5.9878680217,-2.578652816,1.2425210613\C,0,5.4534050024,-3.71404556,0
.372629242\C,0,6.9326364906,-1.6408128336,0.4804731981\O,0,6.727335170
6,-3.1999625503,2.2892039593\O,0,-2.2125047599,0.2566543774,-1.6425986
359\O,0,4.9242328237,-1.5944968712,3.1181776426\H,0,-1.422801664,1.057
9921607,-3.3374059926\H,0,-1.2766532591,2.0934383976,-1.901009825\H,0
,0.910978347,1.1216250441,-2.5798279593\H,0,0.2425805368,-0.5276890722,
-2.3624700356\H,0,4.9928711508,-3.3561567489,-0.5481669885\H,0,4.72191
12625,-4.3084272371,0.9277421191\H,0,6.2964015335,-4.3576604232,0.1048
414086\H,0,6.4537872957,-1.1526127302,-0.3697719251\H,0,7.7727891255,-
2.2355413995,0.110427956\H,0,7.3175702689,-0.8713844501,1.156715435\H,
0,6.6068265936,-2.6622757513,3.0895540803\H,0,-2.1924042116,0.41946207
35,-0.6865227359\H,0,0.4259287559,0.0630829011,3.105799992\C,0,-0.9661
526639,-0.1337836895,1.529231474\H,0,0.2877899083,1.4751402267,2.04302
55578\O,0,-0.9425246523,-1.4389906974,1.2478324309\O,0,-1.9701340763,0
.5437434275,1.3838570426\H,0,-1.8196450674,-1.7130847496,0.9243972314\
H,0,2.6455650465,-0.8061527237,2.9702070209\Version=ES64L-G16RevA.03\
State=1-A\HF=-995.3670814\RMSD=3.908e-09\PG=C01 [X(C14H18O6)]\@
```

Para-

```
1\1\GINC-R771\SP\RM062X TD-FC\6-31+G(d,p)\C12H14O5\ROOT\16-Apr-2019\0\
\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50) s
crf(smd,solvent=h2o) guess=read geom=allcheck maxdisk=2147483648\titl
e\0,1\C,-1.4143802491,1.5708939617,-2.95458373\C,0.028655315,1.239353
3871,-2.6391070409\O,0.7875282573,1.0571283783,-3.8137199142\C,1.14502
96353,2.1556039467,-4.5428806935\C,0.7932563276,3.4670588103,-4.218593
1958\H,0.1887152833,3.7034365362,-3.3507284764\C,1.2293606181,4.510539
1614,-5.0318950755\H,0.9270738424,5.512526871,-4.7558516666\C,2.000500
1771,4.2682080897,-6.1744832071\C,2.3335300202,2.9363521495,-6.4836020
819\H,2.9343879735,2.7304662009,-7.3628904967\C,1.9196735557,1.8914594
703,-5.6795393348\H,2.184784836,0.8647538147,-5.9092803076\C,2.4883502
71,5.3200638503,-7.1063652799\C,2.5015824456,6.8212650748,-6.753248483
4\C,1.0766065446,7.3800455744,-6.8527505405\C,3.1562943824,7.106182724
6,-5.4042695538\O,3.3096010397,7.4786627003,-7.7241754764\O,-2.1057973
068,1.8122375834,-1.8400864744\O,2.9026750196,5.0005245307,-8.21715242
18\O,-1.8890997651,1.5970579917,-4.0699671759\H,0.0442968569,0.2840669
134,-2.1086933128\H,0.4556574821,2.0044128663,-1.9827940997\H,0.392453
3765,6.9374259927,-6.1267722852\H,0.6802511382,7.2057377401,-7.8577883
52\H,1.1216495816,8.4583974119,-6.6747453353\H,2.541645535,6.785862449
,-4.5633289661\H,3.3049338004,8.1869999632,-5.3252233672\H,4.130605230
4,6.6131344854,-5.3398113751\H,3.2525603499,6.9659797976,-8.5472115797
\H,-3.0374025742,1.9918655724,-2.0624676998\Version=ES64L-G16RevA.03\
State=1-A\HF=-841.5612633\RMSD=2.164e-09\PG=C01 [X(C12H14O5)]\@
```

I2959-COO Gas

Ortho-

```
1\1\GINC-R2916\SP\RM062X TD-FC\6-31+G(d,p)\C14H17O6(1-)\ROOT\05-Jan-20
19\0\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-
50) maxdisk=2684354560\title\0,1\C,0,-1.0555426609,1.9432169418,-3.
2829569359\C,0,-1.5471952733,3.1146698685,-4.1084237393\O,0,-1.7240390
571,4.1784531337,-3.1925691237\C,0,-2.1944276968,5.3783908814,-3.67294
39969\C,0,-2.4965696282,5.6084319937,-5.0130497157\H,0,-2.3681915158,4
.8289713126,-5.7560948179\C,0,-2.9720766683,6.8551047993,-5.4442263759
\C,0,-3.2684950207,7.0611676456,-6.9012700123\C,0,-3.1093515339,7.8847
```

846868,-4.4984579892\C,0,-2.8075546597,7.6354275675,-3.1575773988\H,0,
-2.934863374,8.4278616101,-2.4240442532\C,0,-2.3597483327,6.3915791773
, -2.7302174647\H,0,-2.1281369828,6.1933986719,-1.6888671831\C,0,-3.665
7316411,9.2267069124,-4.8999133853\C,0,-2.8731294077,10.5398044528,-4.
6298938555\C,0,-3.6366510373,11.3317079544,-3.5676031605\C,0,-1.418093
6137,10.309075737,-4.2138320833\O,0,-2.9118073319,11.3211574884,-5.803
8581131\O,0,-1.9837881441,1.6034957655,-2.2732663242\O,0,-4.7798424713
,9.2951057683,-5.3784768727\H,0,-0.0785505722,2.1946438973,-2.84622011
45\H,0,-0.9352912415,1.0632488514,-3.9209377973\H,0,-2.5036137624,2.86
79251548,-4.5890478373\H,0,-0.8141172637,3.3838886696,-4.8808560357\H,
0,-3.6593021563,10.8011080096,-2.6089549776\H,0,-4.660271553,11.499014
1496,-3.9112324787\H,0,-3.1420363482,12.2977109863,-3.4244069225\H,0,-
1.3293816885,9.8552746438,-3.2223036003\H,0,-0.9246439011,11.286101805
, -4.1948255503\H,0,-0.9228426447,9.6711168586,-4.9503004372\H,0,-2.576
9980421,10.735532275,-6.5146461254\H,0,-2.2356383801,2.4308254964,-1.8
413659371\H,0,-3.2497960934,6.1083310917,-7.4343328783\C,0,-2.27949608
01,8.0455175376,-7.6136630998\H,0,-4.2643324389,7.5020828064,-7.013238
4025\O,0,-1.9824052956,9.0754147695,-6.9419764053\O,0,-1.9174164867,7.
7299416284,-8.7543735991\\Version=ES64L-G16RevA.03\State=1-A\HF=-994.7
959624\RMSD=4.346e-09\PG=C01 [X(C14H17O6)]\@

Meta-

1\1\GINC-R3504\SP\RM062X TD-FC\6-31+G(d,p)\C14H17O6(1-)\ROOT\05-Jan-20
19\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-
50) maxdisk=2684354560\\title\\-1,1\C,0,-0.9166230304,0.0707941692,-2.
4376198521\C,0,0.3630768098,0.8326586798,-2.747290946\O,0,1.0545266514
,0.2860123959,-3.8722295478\C,0,1.8210295405,-0.8288350195,-3.66025962
06\C,0,1.4740075174,-2.0257416161,-4.296242604\C,0,2.3040093937,-3.131
3673764,-4.1065174464\C,0,0.2035773144,-2.1873636786,-5.0908538122\C,0
,3.4540301779,-3.0719865296,-3.3143978174\C,0,3.7893078986,-1.85120500
89,-2.7042676909\H,0,4.6860231083,-1.7994385768,-2.0959697057\C,0,2.98
07893383,-0.741871739,-2.8789567791\H,0,3.2319116038,0.2072084858,-2.4
14364597\C,0,4.3370571859,-4.2354145181,-3.0506882897\C,0,3.9932569516
, -5.6737169142,-3.5111204894\C,0,2.64845825,-6.1465773827,-2.947356172
9\C,0,4.0557177805,-5.7878196335,-5.0406555869\O,0,4.9965271863,-6.530
1296675,-2.9890650228\O,0,-0.6368468352,-1.1779505,-1.8897710132\O,0,5
.3841055212,-4.0882017331,-2.4288136569\H,0,-1.509440237,-0.0146382226
, -3.3617619632\H,0,-1.4991888771,0.6832145501,-1.72612507\H,0,1.014065
1057,0.8219550425,-1.862967523\H,0,0.142425736,1.8704306328,-3.0201166
024\H,0,1.7814959714,-5.6583138797,-3.3970420488\H,0,2.6220449931,-5.9
881516418,-1.8652305799\H,0,2.5784093087,-7.2221061156,-3.1346855423\H
,0,3.2541565492,-5.248506137,-5.5463742391\H,0,3.9770744223,-6.8490971
8,-5.2933247165\H,0,5.021088153,-5.4202496031,-5.4024082337\H,0,5.6392
636955,-5.9512001425,-2.546042129\H,0,-0.9571464918,-1.9035358684,-2.5
154626569\H,0,-0.360327307,-1.2538825918,-5.0860965086\C,0,-0.62814965
34,-3.3414495944,-4.4577354011\H,0,0.4432650278,-2.4618075922,-6.12290
41717\O,0,-1.4277440336,-2.9997029612,-3.537262312\O,0,-0.3934103475,-
4.4867109938,-4.8823983696\H,0,1.9767016207,-4.0506735376,-4.576464280
8\\Version=ES64L-G16RevA.03\State=1-A\HF=-994.8056572\RMSD=8.599e-09\PG
G=C01 [X(C14H17O6)]\@

Para-

1\1\GINC-R58\SP\RM062X TD-FC\6-31+G(d,p)\C12H13O5(1-)\ROOT\16-Apr-2019
\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50
) guess=read geom=allcheck maxdisk=2147483648\\title\\-1,1\C,-1.042534
9561,2.2105358692,-3.1335944613\C,-0.0235090562,1.2236639393,-2.477799
0093\O,-0.1048947239,1.1069251264,-1.0534097407\C,-1.1953688188,0.5656
992875,-0.5152720839\C,-2.2890253089,0.0679976873,-1.2453352158\H,-2.3
340482573,0.1917840347,-2.3195115505\C,-3.3448395094,-0.5300053837,-0.
5762674639\H,-4.1720920378,-0.8855789991,-1.1773091818\C,-3.3624386962
, -0.6609693116,0.8233965454\C,-2.2613635809,-0.1468364601,1.5378906461
\H,-2.2658088263,-0.2348985453,2.619352529\C,-1.2030952835,0.452653637
4,0.8896133548\H,-0.3560017043,0.8532125565,1.4363482233\C,-4.44084649
65,-1.2867237846,1.609367718\C,-5.7278493228,-1.875633004,0.9728859838
\C,-6.5485797661,-0.7846449982,0.2762527842\C,-5.4042697281,-3.0534140

779,0.046511198\O,-6.5238122406,-2.3886965677,2.0253967522\O,-1.778175
7021,2.8488667581,-2.3593782791\O,-4.3615147782,-1.3669352248,2.833611
2141\O,-0.960820538,2.202676274,-4.3810444175\H,0.9880076948,1.5850775
294,-2.669330806\H,-0.128572938,0.230677617,-2.9325038367\H,-6.0552690
943,-0.3648611138,-0.601142771\H,-6.753255034,0.0265765552,0.980529842
\H,-7.5038810386,-1.2237501457,-0.0266050374\H,-4.8641457675,-2.759931
7282,-0.8542433704\H,-6.350001668,-3.5216575395,-0.2422953812\H,-4.807
7175164,-3.793897953,0.5871703027\H,-6.0262363062,-2.2055130346,2.8419
865127\Version=ES64L-G16RevA.03\State=1-A\HF=-841.0024279\RMSD=2.062e
-09\PG=C01 [X(C12H13O5)]\@

I2959-COO Toluene

Ortho-

1\1\GINC-R2217\SP\RM062X TD-FC\6-31+G(d,p)\C14H17O6(1-)\ROOT\05-Jan-20
19\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=
toluene) td(nstates=10,50-50) maxdisk=2684354560\title\ -1,1\C,0,-1.0
143477647,1.967367814,-3.2809338037\C,0,-1.5259809159,3.1280754772,-4.
1054145237\O,-1.7430044926,4.1906412574,-3.1878930505\C,0,-2.2174459
502,5.37954929,-3.6681986857\C,0,-2.5084926743,5.6116769038,-5.0119575
614\H,0,-2.3699361411,4.8313561926,-5.7522443928\C,0,-2.9857165613,6.8
568204243,-5.44377037\C,0,-3.2881654235,7.0526114435,-6.9034812241\C,0
, -3.1351410376,7.8863992478,-4.5003093509\C,0,-2.8500896495,7.63532241
43,-3.1545330117\H,0,-2.9883865988,8.4239157705,-2.419118023\C,0,-2.40
47532332,6.3920879817,-2.7259307364\H,0,-2.1884157141,6.1945726366,-1.
6810300904\C,0,-3.6524453065,9.2355920112,-4.9203894519\C,0,-2.8411476
719,10.5314511753,-4.6223755473\C,0,-3.6198563468,11.3438359232,-3.589
1042596\C,0,-1.4069577207,10.2725859792,-4.1584806041\O,0,-2.817903610
3,11.3055087449,-5.8054691075\O,0,-1.9551358177,1.5732619544,-2.299984
866\O,0,-4.7377477556,9.3300860569,-5.4597695279\H,0,-0.0577741536,2.2
445651789,-2.8161087839\H,0,-0.8454578191,1.1041150717,-3.9303289186\H
0,0,-2.4690529526,2.8595253228,-4.5993754438\H,0,-0.7868725055,3.417276
6709,-4.8639391968\H,0,-3.6975155443,10.8122769137,-2.6342794371\H,0,-
4.6256720497,11.5471405317,-3.9655309158\H,0,-3.1048175496,12.29477693
14,-3.4178388919\H,0,-1.3567498598,9.8331086388,-3.1585408766\H,0,-0.8
876593672,11.2361544997,-4.1360701758\H,0,-0.8986335562,9.6125534731,-
4.8664541319\H,0,-2.4796596481,10.7035203848,-6.499907009\H,0,-2.20808
91498,2.3692857654,-1.8133843054\H,0,-3.2301362555,6.0985826015,-7.432
0024614\C,0,-2.3746288763,8.073346582,-7.6463273296\H,0,-4.3081950927,
7.4344331352,-7.0198905447\O,0,-1.9330093843,9.0336752298,-6.952988139
6\O,0,-2.196375849,7.8591353695,-8.8568702494\Version=ES64L-G16RevA.0
3\State=1-A\HF=-994.8519731\RMSD=5.880e-09\PG=C01 [X(C14H17O6)]\@

Meta-

1\1\GINC-R3339\SP\RM062X TD-FC\6-31+G(d,p)\C14H17O6(1-)\ROOT\05-Jan-20
19\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=
toluene) td(nstates=10,50-50) maxdisk=2684354560\title\ -1,1\C,0,-0.6
119352215,1.6484843839,-2.7295694212\C,0,0.4296031011,0.565095769,-2.9
582473641\O,0,1.5428791646,1.1624461492,-3.6248437301\C,0,2.8025857163
,0.9039848666,-3.2258899828\C,0,3.74885617,1.9112771808,-3.5094791079\
C,0,5.0655772834,1.6931705505,-3.1342735648\C,0,3.2947482664,3.1807068
901,-4.1675830707\C,0,5.4817299818,0.5061230755,-2.500575925\C,0,4.517
8329336,-0.4790752864,-2.2504797086\H,0,4.8267707636,-1.4024489832,-1.
772281646\C,0,3.1900858033,-0.2897422767,-2.6072640824\H,0,2.461911861
6,-1.0700418911,-2.4151348294\C,0,6.8716008457,0.2103952356,-2.0751907
233\C,0,8.0462640399,1.2041298616,-2.2520099692\C,0,8.3256325939,1.470
923113,-3.7352110439\C,0,7.8106490225,2.4899867937,-1.4534940042\O,0,9
.2060179324,0.5878181062,-1.7176927829\O,0,-0.300444213,2.4870443465,-
1.6555235495\O,0,7.1414284059,-0.8662897923,-1.5518371012\H,0,-1.56574
2559,1.1562616502,-2.498826758\H,0,-0.7425041173,2.2097041717,-3.66841
86812\H,0,0.0347492088,-0.2432205974,-3.587931877\H,0,0.7364974499,0.1
600484098,-1.9884538784\H,0,7.5322826665,2.0296847265,-4.2334728414\H,
0,8.4715135469,0.5239479799,-4.2640510842\H,0,9.2538811379,2.046073523
9,-3.8040912337\H,0,6.9869495424,3.0947031643,-1.8348055266\H,0,8.7287
405483,3.0841235721,-1.4927926411\H,0,7.6057182833,2.2474518895,-0.406

4847433\H,0,8.9234786383,-0.2851347288,-1.3955719412\H,0,0.5328478917,
2.9952734457,-1.8521467134\H,0,4.1476615561,3.8565135517,-4.2976919129
\C,0,2.1888574287,3.9610915734,-3.3963299367\H,0,2.8937688303,2.977649
8781,-5.1660378863\O,0,2.0253485982,3.6592725138,-2.1796039784\O,0,1.5
827713682,4.8242373729,-4.056213142\H,0,5.7711035292,2.4889738104,-3.3
397316169\\Version=ES64L-G16RevA.03\State=1-A\HF=-994.8590249\RMSD=4.5
03e-09\PG=C01 [X(C14H17O6)]\@

Para-

1\1\GINC-R56\SP\RM062X TD-FC\6-31+G(d,p)\C12H13O5(1-)\ROOT\16-Apr-2019
\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50
) scrf(smd,solvent=toluene) guess=read geom=allcheck maxdisk=214748364
8\\title\\-1,1\C,-1.2465233078,2.0247094796,-3.0001597519\C,0.00193398
39,1.3036147115,-2.4163784222\O,-0.0142157206,1.097989055,-1.003698471
3\C,0.0482489736,2.1672810792,-0.2037661997\C,0.1720857181,3.491550503
7,-0.6512351814\H,0.1644645082,3.7236161894,-1.709000275\C,0.257272236
6,4.5248454433,0.2717200016\H,0.3355198455,5.5312448327,-0.118795096\C
,0.2326741906,4.2853340552,1.6540518749\C,0.111716523,2.9484773944,2.0
831648367\H,0.0884047957,2.7468017949,3.1489348576\C,0.0210970496,1.91
00878061,1.1797300924\H,-0.0798909162,0.8814495184,1.5103656362\C,0.31
55433349,5.3268964426,2.7018628236\C,0.4007919363,6.8431460364,2.39371
5286\C,1.6937748034,7.188071798,1.6467104601\C,-0.8523751709,7.3306971
193,1.6597716337\O,0.448276696,7.5234510819,3.6365314651\O,-2.21668043
23,2.1953927717,-2.2377689837\O,0.3139808315,5.011479543,3.888499459\O
, -1.1026695531,2.3298682118,-4.207178127\H,0.9122731524,1.8436180949,-
2.7030473328\H,0.0529172665,0.2999102696,-2.8445344057\H,1.7265794041,
6.7954125446,0.6295105679\H,2.558070474,6.8042421881,2.1973342741\H,1.
7753415294,8.2783582146,1.6015037067\H,-0.9430413731,6.9380528198,0.64
6046697\H,-0.8104355616,8.4229889008,1.6093093856\H,-1.7481455078,7.04
88060162,2.221258583\H,0.4131122901,6.8341690833,4.3219186055\\Version
=ES64L-G16RevA.03\State=1-A\HF=-841.0581859\RMSD=5.962e-09\PG=C01 [X(C
12H13O5)]\@

I2959-COO DCM

Ortho-

1\1\GINC-R2375\SP\RM062X TD-FC\6-31+G(d,p)\C14H17O6(1-)\ROOT\05-Jan-20
19\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=
dichloromethane) td(nstates=10,50-50) maxdisk=2684354560\\title\\-1,1\
C,0,-1.0588305283,1.9424225826,-3.2526833484\C,0,-1.52172575,3.1138660
079,-4.088532179\O,0,-1.7072940721,4.1982876995,-3.1830864676\C,0,-2.1
706507477,5.3828247266,-3.6696228116\C,0,-2.4499415288,5.6130390526,-5
.0184110646\H,0,-2.3048240881,4.8290371153,-5.7536428672\C,0,-2.929876
7316,6.8559144434,-5.4530066608\C,0,-3.2429071905,7.0381755815,-6.9157
529011\C,0,-3.0914295355,7.88556662,-4.5108391258\C,0,-2.8072064508,7.
6422772241,-3.1622114504\H,0,-2.9516643546,8.4333571709,-2.4309886176\
C,0,-2.3618254823,6.4006027702,-2.7308474634\H,0,-2.1524593089,6.20648
84467,-1.6836716132\C,0,-3.6222751732,9.2219845671,-4.9401306744\C,0,-
2.8511744801,10.5348493428,-4.6224820096\C,0,-3.6554112029,11.31532021
47,-3.5855317107\C,0,-1.4135694003,10.3137778998,-4.1534367813\O,0,-2.
8428128284,11.3170892569,-5.8069878508\O,0,-2.0354839131,1.561351798,-
2.298282561\O,0,-4.689161215,9.2926778923,-5.5228746917\H,0,-0.1094347
541,2.1934703674,-2.7608542162\H,0,-0.8940617405,1.0798008623,-3.90327
60417\H,0,-2.4705757842,2.8766578784,-4.5858961055\H,0,-0.7667343436,3
.3688873525,-4.8428209444\H,0,-3.7244962185,10.7643795534,-2.641887043
3\H,0,-4.6645790835,11.5043500257,-3.9616727317\H,0,-3.161502974,12.27
34742776,-3.3939908026\H,0,-1.36186058,9.8620185392,-3.1599626413\H,0,
-0.9226096101,11.2911666488,-4.1101677686\H,0,-0.8771781657,9.67808349
89,-4.8632500218\H,0,-2.4815392306,10.7294425945,-6.5002697687\H,0,-2.
2197947954,2.3305330103,-1.7409038576\H,0,-3.0900668488,6.0950930917,-
7.4460613619\C,0,-2.4518644958,8.1387087477,-7.6721459095\H,0,-4.29869
33727,7.3054252983,-7.0365225098\O,0,-1.9138719213,9.050044556,-6.9816
709031\O,0,-2.441982099,8.0357442848,-8.9158495221\\Version=ES64L-G16R
evA.03\State=1-A\HF=-994.8826201\RMSD=3.645e-09\PG=C01 [X(C14H17O6)]\@
@

Meta-

```
1\1\GINC-R3452\SP\RM062X TD-FC\6-31+G(d,p)\C14H17O6(1-)\ROOT\05-Jan-20
19\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=
dichloromethane) td(nstates=10,50-50) maxdisk=2684354560\title\ -1,1\C,
0,-1.0719566967,1.4285338577,-2.4337905734\C,0,0.2724174847,0.769924
7104,-2.1964034662\O,0,0.4592435504,0.7751191555,-0.7838142369\C,0,1.4
241476106,0.024791945,-0.2192887451\C,0,1.2815243746,-0.1622688711,1.1
717314677\C,0,2.2383580297,-0.9143844674,1.8351964826\C,0,0.0633775061
,0.4120804037,1.8426868976\C,0,3.3308987136,-1.4907511046,1.1566283478
\C,0,3.4338849308,-1.2916750006,-0.2263701118\H,0,4.2685822744,-1.7343
664578,-0.7596106964\C,0,2.493384457,-0.5390672674,-0.9198681767\H,0,2
.5926632756,-0.3952578298,-1.9901511405\C,0,4.3903868261,-2.3125023042
,1.7979736905\C,0,4.4942874041,-2.5246203537,3.3263031749\C,0,4.632021
3755,-1.1972594323,4.0758380699\C,0,3.3220857027,-3.3727650878,3.83416
33294\O,0,5.6866237786,-3.2555396205,3.5716548801\O,0,-2.1384781298,0.
6788574273,-1.9053277451\O,0,5.2427502239,-2.8605775704,1.1062716668\H
,0,-1.2288984066,1.5160326827,-3.5142080247\H,0,-1.047618228,2.4442254
8,-2.0117093194\H,0,1.076015063,1.3313150799,-2.6908026958\H,0,0.26513
20299,-0.2642500941,-2.5622233869\H,0,3.7199117565,-0.5994294959,4.062
2070973\H,0,5.4479588547,-0.6059311386,3.6487359952\H,0,4.880073822,-1
.424641562,5.1170297522\H,0,2.3569224347,-2.8702640696,3.7555690925\H,
0,3.5073244922,-3.6066361909,4.8869873335\H,0,3.2721247225,-4.31247812
98,3.2753308286\H,0,6.0330312798,-3.5249740287,2.703776857\H,0,-2.1014
621686,0.6857858571,-0.9206390011\H,0,0.0869668393,0.1636033455,2.9091
555714\C,0,-1.2423789823,-0.1689398054,1.2327700143\H,0,0.0431073076,1
.5004762168,1.7388162351\O,0,-1.3161667573,-1.4138383912,1.1617910893\
O,0,-2.1219148596,0.6643107183,0.8667319722\H,0,2.0993371084,-1.062396
606,2.8991204742\Version=ES64L-G16RevA.03\State=1-A\HF=-994.8892073\R
MSD=7.261e-09\PG=C01 [X(C14H17O6)]\@
```

Para-

```
1\1\GINC-R62\SP\RM062X TD-FC\6-31+G(d,p)\C12H13O5(1-)\ROOT\16-Apr-2019
\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50
) scrf(smd,solvent=dichloromethane) guess=read geom=allcheck maxdisk=2
147483648\title\ -1,1\C,-1.2868490692,1.9559433908,-2.9905980009\C,0.
0057593634,1.3135723044,-2.4308652783\O,0.0096777794,1.1085222382,-1.0
215410268\C,0.0617412075,2.1813098956,-0.2156318683\C,0.1771118596,3.5
055749457,-0.6601707961\H,0.1885266388,3.7429183423,-1.7171470196\C,0.
2532682832,4.5394629724,0.2665160587\H,0.3349003836,5.5460922694,-0.12
22593901\C,0.2182611545,4.2933338728,1.6464217621\C,0.0998198635,2.955
2947335,2.0719846203\H,0.0677726047,2.7466479043,3.13625044\C,0.023767
7925,1.9171835981,1.165061902\H,-0.069525923,0.8874841084,1.4955208405
\C,0.2920623583,5.3333695981,2.7023037355\C,0.4096000179,6.8466143388,
2.4039744299\C,1.7160990543,7.1696467875,1.6718721247\C,-0.827631655,7
.3603237617,1.6605036294\O,0.4577169114,7.5209808182,3.6524874079\O,-2
.2560793747,2.0848938483,-2.2142727775\O,0.2586851188,5.0059111745,3.8
847077242\O,-1.2053648485,2.2556988784,-4.2075165272\H,0.878837396,1.9
036194232,-2.7322153466\H,0.106651071,0.3143756282,-2.8614731952\H,1.7
470512185,6.784404638,0.6519204909\H,2.5672617898,6.7631319648,2.22695
11275\H,1.8183928812,8.2583907283,1.6332364226\H,-0.9109998927,6.97516
4142,0.6433013444\H,-0.7625461947,8.4516308346,1.6136417243\H,-1.73439
68698,7.0920969537,2.2114594543\H,0.3905310796,6.8379689059,4.34195398
72\Version=ES64L-G16RevA.03\State=1-A\HF=-841.0877171\RMSD=4.517e-09\
PG=C01 [X(C12H13O5)]\@
```

I2959-COO Acetonitrile

Ortho-

```
1\1\GINC-R1821\SP\RM062X TD-FC\6-31+G(d,p)\C14H17O6(1-)\ROOT\05-Jan-20
19\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=
acetonitrile) td(nstates=10,50-50) maxdisk=2684354560\title\ -1,1\C,0
,-1.2520694062,2.2411962635,-2.6305060695\C,0,-0.0283906109,1.40469468
3,-2.3347528232\O,0,0.0708364246,1.3340468515,-0.9137830395\C,0,1.0618
302891,0.5772277575,-0.371473435\C,0,1.0731249494,0.499133707,1.027463
2291\H,0,0.3029055307,1.0318048034,1.579430637\C,0,2.0296718662,-0.248
```

4755794,1.7078568956\C,0,1.9535236197,-0.3493370123,3.2104188068\C,0,3
.0289118838,-0.9019046828,0.9526322733\C,0,3.0126524801,-0.8169874918,
-0.4375714023\H,0,3.7722512889,-1.3356024624,-1.0171520919\C,0,2.02968
63167,-0.0946174296,-1.1180702874\H,0,2.0392718259,-0.059974007,-2.200
8529589\C,0,4.067271516,-1.727329596,1.651673372\C,0,5.5860642221,-1.4
73804696,1.431247525\C,0,6.1607142614,-2.6732421065,0.6833113496\C,0,5
.8991544239,-0.1690011338,0.7003667533\O,0,6.1982330881,-1.4497844387,
2.7132091046\O,0,-2.4334033549,1.6389247624,-2.1265847319\O,0,3.721969
0599,-2.6204424327,2.4048245399\H,0,-1.3726180281,2.3282658361,-3.7131
474439\H,0,-1.1196328566,3.2483112145,-2.2133031744\H,0,0.867942612,1.
8741599652,-2.7584949937\H,0,-0.1437573732,0.3953955537,-2.7492268218\
H,0,5.711217335,-2.766763868,-0.3105269171\H,0,5.9716648218,-3.5911881
859,1.2464322694\H,0,7.2413343384,-2.5421071473,0.5667227258\H,0,5.588
9681358,-0.1921641952,-0.3468617521\H,0,6.9830989455,-0.0199977774,0.7
322881957\H,0,5.4103118616,0.6725427187,1.1994136148\H,0,5.6974650578,
-0.7793505429,3.222900106\H,0,-2.32133768,1.5266109783,-1.1725620195\
H,0,1.1766476094,0.3290199579,3.5783674653\C,0,3.2385933002,-0.04865145
23,4.0199885605\H,0,1.6442056753,-1.3596966275,3.4973878156\O,0,4.2634
97755,0.3380148185,3.3863112911\O,0,3.1438618156,-0.2118030055,5.25437
04318\Version=ES64L-G16RevA.03\State=1-A\HF=-994.890047\RMSD=4.625e-0
9\PG=C01 [X(C14H17O6)]\@

Meta-

1\1\GINC-R157\SP\RM062X TD-FC\6-31+G(d,p)\C14H17O6(1-)\ROOT\05-Jan-201
9\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=a
cetonitrile) td(nstates=10,50-50) maxdisk=2684354560\title\ -1,1\C,0,
-1.1070795748,1.3011554729,-2.4798874383\C,0,0.2476192722,0.6715320562
, -2.227629943\O,0,0.4426001076,0.7326124985,-0.8163573992\C,0,1.433412
0824,0.0316555315,-0.2337797529\C,0,1.3142377663,-0.0980319106,1.16599
65967\C,0,2.2939878227,-0.8028023258,1.8484953122\C,0,0.0996702955,0.4
892926954,1.8327183996\C,0,3.3928809487,-1.3794330689,1.1804447349\C,0
,3.477252069,-1.2308284199,-0.2103904009\H,0,4.3161396609,-1.673720085
3,-0.7368780765\C,0,2.5076384466,-0.5356510433,-0.9241106789\H,0,2.589
5558391,-0.4384366086,-2.0011482116\C,0,4.479865323,-2.1513902879,1.83
99924283\C,0,4.4595376149,-2.5449103545,3.3350930334\C,0,4.6007542301,
-1.302597407,4.2224481234\C,0,3.2257097142,-3.3810538785,3.6834064979\
O,0,5.5936927955,-3.3668364134,3.5706748461\O,0,-2.1578345375,0.569487
7887,-1.8917440063\O,0,5.4530347195,-2.5137569977,1.1867533996\H,0,-1.
2817455317,1.327001689,-3.5603350866\H,0,-1.0898445065,2.3384607373,-2
.1146155974\H,0,1.0390427911,1.2249767642,-2.7486947086\H,0,0.25549062
75,-0.3758063946,-2.5539096865\H,0,3.7368396435,-0.6381493814,4.173660
8336\H,0,5.4946318388,-0.7388742456,3.9372308565\H,0,4.7195590599,-1.6
400615587,5.2565492997\H,0,2.2990785872,-2.8059380103,3.6617116461\H,0
,3.3626795733,-3.7745097861,4.695203791\H,0,3.1340013038,-4.2254652904
,2.9932347595\H,0,6.1173536817,-3.361636017,2.7512363553\H,0,-2.097544
8355,0.6272801012,-0.9110240553\H,0,0.1427866608,0.2806608889,2.907149
7519\C,0,-1.2107948948,-0.1213958995,1.2675328986\H,0,0.0697179036,1.5
732532674,1.6907981362\O,0,-1.2793348606,-1.369469355,1.2414935689\O,0
, -2.1053230191,0.6903614778,0.8897493418\H,0,2.1764003812,-0.896734229
,2.9211934307\Version=ES64L-G16RevA.03\State=1-A\HF=-994.8963369\RMSD
=7.196e-09\PG=C01 [X(C14H17O6)]\@

Para-

1\1\GINC-R63\SP\RM062X TD-FC\6-31+G(d,p)\C12H13O5(1-)\ROOT\16-Apr-2019
\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50
) scrf(smd,solvent=acetonitrile) guess=read geom=allcheck maxdisk=2147
483648\title\ -1,1\C,-1.3013640291,1.946196273,-2.9853725359\C,-0.000
3804603,1.3153671591,-2.4343202123\O,0,0.0132577012,1.1107591174,-1.0253
08062\C,0,0.0677149564,2.1839028638,-0.2188024527\C,0.1911604524,3.50778
72555,-0.662103285\H,0.2137645542,3.7463546485,-1.7187194562\C,0.26827
54324,4.5416651695,0.2653839798\H,0.360205269,5.5473620676,-0.12355723
45\C,0.2243965076,4.2945956184,1.644898019\C,0.0994657887,2.9568436719
,2.069240837\H,0.0626590073,2.7460459649,3.1329424637\C,0.023057302,1.
9189992385,1.1614288569\H,-0.073570069,0.8896591163,1.4924986366\C,0.2
96028428,5.3341411769,2.7029463974\C,0.4059984859,6.8476581769,2.40667

89119\C,1.7163655345,7.176988854,1.6843953348\C,-0.8272710708,7.354952
4572,1.652834333\O,0.4384345929,7.5208838292,3.6568617206\O,-2.2643535
964,2.0814820821,-2.2008392722\O,0.2654992069,5.0030536522,3.884319012
1\O,-1.2377823527,2.2315089983,-4.206961359\H,0.8658957967,1.911518571
8,-2.7424647682\H,0.1053353818,0.3169060353,-2.865544433\H,1.755097621
,6.7922128638,0.664544645\H,2.5655668025,6.7742487971,2.2452847453\H,1
.8129570867,8.2662266713,1.6454330249\H,-0.8946325845,6.9746120444,0.6
326698117\H,-0.7691061447,8.4468242033,1.6106648326\H,-1.7381467043,7.
0775287625,2.1925353189\H,0.3855731037,6.8352776591,4.3448101897\\Vers
ion=ES64L-G16RevA.03\State=1-A\HF=-841.0942954\RMSD=3.925e-09\PG=C01 [X
(C12H13O5)]\@

I2959-COO Water

Ortho-

1\1\GINC-R3177\SP\RM062X TD-FC\6-31+G(d,p)\C14H17O6(1-)\ROOT\05-Jan-20
19\O\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=
h2o) td(nstates=10,50-50) maxdisk=2684354560\\title\\-1,1\C,0,-1.62002
39564,1.9354454086,-2.6835089208\C,0,-1.8677803171,3.007811746,-3.7172
647775\O,0,-2.0303742453,4.2360161937,-3.0055159264\C,0,-2.3320923284,
5.3573285418,-3.7194968251\C,0,-2.5455690043,6.517743141,-2.9652754016
\H,0,-2.4695471218,6.4536035604,-1.8832583309\C,0,-2.8383060719,7.7328
558035,-3.5742602413\C,0,-2.9963567882,8.9627491609,-2.7128374053\C,0,
-2.9595166159,7.7642289109,-4.9811509272\C,0,-2.7595626201,6.601209803
3,-5.7234981013\H,0,-2.8402321095,6.6337246334,-6.8065371888\C,0,-2.42
7570785,5.3933170813,-5.1109505427\H,0,-2.2575749137,4.5118397299,-5.7
168374305\C,0,-3.2742678561,9.0539001093,-5.6612257585\C,0,-4.45106205
21,9.178184138,-6.6628201901\C,0,-3.8648570058,9.3374872037,-8.0624842
329\C,0,-5.448305236,8.0238984227,-6.6131022887\O,0,-5.1242274009,10.3
983273938,-6.351579056\O,0,-2.739162509,1.7596852587,-1.8229404854\O,0
-2.6088002405,10.051790282,-5.4178876444\H,0,-0.7230135935,2.17879654
27,-2.1015731659\H,0,-1.4574150777,0.9837341176,-3.1940640517\H,0,-2.7
788985286,2.7902357605,-4.2869275079\H,0,-1.0144130451,3.0774685676,-4
.4019492852\H,0,-3.3031645367,8.4433703993,-8.3479150648\H,0,-3.197718
2607,10.2029359877,-8.0983495119\H,0,-4.6801467143,9.482273034,-8.7776
904729\H,0,-5.0225817783,7.0975425275,-7.003018397\H,0,-6.3033198218,8
.2948122222,-7.2392704809\H,0,-5.8000860634,7.8489386279,-5.5929010987
\H,0,-5.3943437242,10.3309311503,-5.415285753\H,0,-2.8680048489,2.5802
128344,-1.3267033955\H,0,-3.0862620351,8.6549510526,-1.665170499\C,0,-
4.1952913312,9.8785560448,-3.0005199576\H,0,-2.0969002617,9.5827579191
, -2.7750963975\O,0,-5.153683406,9.4338158597,-3.6963396096\O,0,-4.1478
30795,11.0300008294,-2.4926146754\\Version=ES64L-G16RevA.03\State=1-A\
HF=-994.9067272\RMSD=2.554e-09\PG=C01 [X(C14H17O6)]\@

Meta-

1\1\GINC-R2193\SP\RM062X TD-FC\6-31+G(d,p)\C14H17O6(1-)\ROOT\05-Jan-20
19\O\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=
h2o) td(nstates=10,50-50) maxdisk=2684354560\\title\\-1,1\C,0,-1.15167
39926,1.1731152793,-2.4179167614\C,0,0.2569671392,0.6761129554,-2.1827
145065\O,0,0.4543017166,0.7152836947,-0.7672868082\C,0,1.5260758634,0.
0959010179,-0.2227491302\C,0,1.4451586335,-0.1051590964,1.171639886\C,
0,2.5072377834,-0.7241480662,1.8048919495\C,0,0.1941734382,0.332087883
1,1.8867499209\C,0,3.6452419008,-1.1603004722,1.0957767235\C,0,3.68882
42346,-0.955847654,-0.2878641351\H,0,4.5420736241,-1.2606096088,-0.879
7565418\C,0,2.6378446206,-0.3253252698,-0.9503891423\H,0,2.6958420759,
-0.1630430261,-2.0204504818\C,0,4.7241822676,-1.8037736052,1.887581493
7\C,0,5.8749783055,-2.6114078509,1.2514331689\C,0,5.3726350692,-3.6942
998422,0.2993624436\C,0,6.8752847268,-1.6551870511,0.5898759612\O,0,6.
5471609645,-3.2928627923,2.3065750107\O,0,-2.122282847,0.3130699914,-1
.8394218662\O,0,4.7238926934,-1.703218282,3.1126716064\H,0,-1.33909984
8,1.2026953823,-3.4942439477\H,0,-1.2520344734,2.19087189,-2.020449457
1\H,0,0.9848429754,1.32246201,-2.686197055\H,0,0.3709812605,-0.3553040
633,-2.535922895\H,0,4.9619553285,-3.2841723925,-0.6233010314\H,0,4.60
73594478,-4.3051319624,0.7870178933\H,0,6.2202811079,-4.3357931532,0.0
411306859\H,0,6.4537399977,-1.118771761,-0.2615031057\H,0,7.7266951861

, -2.2461382308, 0.2398978963\H, 0, 7.231942974, -0.9255734798, 1.3233247838
\H, 0, 6.3612233468, -2.8081010979, 3.1283186773\H, 0, -2.0783801988, 0.38924
7885, -0.8650640884\H, 0, 0.2508285013, 0.0265199941, 2.9364421902\C, 0, -1.0
630825582, -0.3040274906, 1.2710744343\H, 0, 0.089064201, 1.4200744485, 1.85
25551125\O, 0, -1.04122264, -1.5447826068, 1.0604024504\O, 0, -2.0487480888,
0.4533177945, 1.017210882\H, 0, 2.4547802624, -0.8967343708, 2.8757497836\|
Version=ES64L-G16RevA.03\State=1-A\HF=-994.91288\RMSD=4.626e-09\PG=C01
[X(C14H17O6)]\|@

Para-

1\1\GINC-R54\SP\RM062X TD-FC\6-31+G(d,p)\C12H13O5(1-)\ROOT\16-Apr-2019
\0\|# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50
) scrf(smd,solvent=h2o) guess=read geom=allcheck maxdisk=2147483648\|t
itle\|-1,1\C, -1.4149568688, 1.735794102, -2.7823738031\C, 0.03912953, 1.30
94894224, -2.5333684201\O, 0.7876978761, 1.0894472608, -3.7213096463\C, 1.1
417704874, 2.1657423839, -4.4695918454\C, 0.8415893588, 3.4901458532, -4.13
57646905\H, 0.276918405, 3.7373059234, -3.244640637\C, 1.269291916, 4.52020
47017, -4.9684612975\H, 1.0062444785, 5.530002844, -4.6810775178\C, 1.98482
25375, 4.2578264241, -6.1438374135\C, 2.2687891095, 2.9160559815, -6.462441
2005\H, 2.8251139073, 2.6930361, -7.3665670048\C, 1.8620205409, 1.883526531
3, -5.6397486985\H, 2.088992682, 0.8501233078, -5.8806523463\C, 2.457885337
2, 5.2937008462, -7.0970699051\C, 2.4801590176, 6.8004399238, -6.7664972121
\C, 1.0514706431, 7.3565977991, -6.8065163421\C, 3.1972997223, 7.1040010244
, -5.4531914145\O, 3.2376691498, 7.4470878456, -7.784865448\O, -2.048634442
4, 2.0770627811, -1.7464420478\O, 2.8524154384, 4.9600380328, -8.212231715\
O, -1.8643932531, 1.687512509, -3.9537362863\H, 0.0241279738, 0.346517239, -
2.017893881\H, 0.5388275773, 2.0375463284, -1.8868030426\H, 0.4055930471, 6
.9325197093, -6.0361210377\H, 0.6042444738, 7.1587156695, -7.7854635925\H,
1.1047225486, 8.4389441037, -6.6571217983\H, 2.6277051998, 6.7877942298, -4
.5796070889\H, 3.3420042385, 8.1865756018, -5.3922631589\H, 4.1772995279, 6
.6184330595, -5.4322878718\H, 3.1890988398, 6.8906164612, -8.5799906361\|
Version=ES64L-G16RevA.03\State=1-A\HF=-841.1097078\RMSD=2.163e-09\PG=C0
1 [X(C12H13O5)]\|@

I2959-NMe₂ Gas

Ortho-

1\1\GINC-R47\SP\RM062X TD-FC\6-31+G(d,p)\C15H23N1O4\ROOT\21-Jan-2019\0
\|# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50)
maxdisk=2684354560\|title\|0,1\C, 0, 2.2991905655, -4.4840068762, -2.93376
5152\C, 0, 1.9529105065, -3.0531299676, -2.5769408702\O, 0, 1.8956321799, -3.
0068274868, -1.1577196652\C, 0, 1.6599534325, -1.8101505864, -0.5563208199\
C, 0, 1.6480681235, -1.8237901205, 0.8450931247\C, 0, 1.4076139521, -0.665370
8988, 1.5644424423\C, 0, 1.4129996362, -0.6636662451, 3.0768691755\C, 0, 1.19
53439766, 0.5490766328, 0.878648307\C, 0, 1.2225251696, 0.553705624, -0.5108
48634\H, 0, 1.0452488646, 1.473666567, -1.0574950811\C, 0, 1.4442833235, -0.6
174061087, -1.2415211317\H, 0, 1.4455225269, -0.5781477737, -2.3236858575\C
0, 0.8808796388, 1.7826806587, 1.6778639229\C, 0, 1.7065210889, 3.077255228
7, 1.5298016581\C, 0, 3.1924057486, 2.8113908164, 1.3333938655\C, 0, 1.128757
5628, 3.9098236801, 0.371081977\O, 0, 1.5594368932, 3.8137123423, 2.72741710
23\O, 0, 3.5573660385, -4.8522544292, -2.415414829\O, 0, -0.0696930869, 1.793
0799793, 2.4401678671\H, 0, 2.3599294133, -4.5842506199, -4.020419894\H, 0, 1
.5064487215, -5.1507265295, -2.5672811106\H, 0, 0.9843347324, -2.7637939509
, -3.0063216321\H, 0, 2.7350624316, -2.3735529499, -2.9391701134\H, 0, 3.3819
994429, 2.270212387, 0.4026403744\H, 0, 3.5732306203, 2.2268702963, 2.172594
4154\H, 0, 3.716855352, 3.7704521992, 1.2996329643\H, 0, 1.3370933942, 3.4732
345313, -0.6087781286\H, 0, 1.5963516951, 4.8971751214, 0.4123969632\H, 0, 0.
0479971893, 4.0331630469, 0.4884804524\H, 0, 0.7086026498, 3.5547899624, 3.1
140820441\H, 0, 3.5349954801, -4.7064901306, -1.4613547712\H, 0, 0.408691228
5, -0.4179636751, 3.4332769277\N, 0, 2.3325218839, 0.3542172832, 3.571758980
7\H, 0, 1.6674627859, -1.6700666412, 3.4552973686\C, 0, 3.7125533035, -0.0902
339785, 3.4806432901\C, 0, 1.9908628081, 0.8040318644, 4.9096953698\H, 0, 3.9
111540097, -0.9692855283, 4.12130968\H, 0, 4.3817703708, 0.7179278237, 3.789
730859\H, 0, 3.9486976779, -0.3563006761, 2.4452503265\H, 0, 2.0499376214, -0
.0056848736, 5.6598054389\H, 0, 0.973621758, 1.2064011468, 4.9024403565\H, 0

,2.6746255835,1.604134691,5.2060955452\H,0,1.8360247048,-2.764059836,1.3556638914\\Version=ES64L-G16RevA.03\State=1-A\HF=-940.7205642\RMSD=6.315e-09\PG=C01 [X(C15H23N1O4)]\\@

Meta-

1\1\GINC-R62\SP\RM062X TD-FC\6-31+G(d,p)\C15H23N1O4\ROOT\21-Jan-2019\0
\\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50)
maxdisk=2684354560\\title\\0,1\C,0,4.2956354134,2.1481680401,3.4490812
041\C,0,4.6420796433,0.9051523752,2.6489964651\O,0,3.4717891174,0.0838
232588,2.6880719373\C,0,2.9993395313,-0.4711341901,1.550629823\C,0,1.5
993234392,-0.5865529833,1.4515448084\C,0,1.0651490923,-1.1918032092,0.
3262286985\C,0,0.7328227688,-0.0251558577,2.5502000813\C,0,1.873610752
,-1.6820904045,-0.7139908256\C,0,3.2601186415,-1.5451846953,-0.5926101
186\H,0,3.9282152265,-1.9082666836,-1.3624144341\C,0,3.8237297119,-0.9
470235142,0.5304822315\H,0,4.9016525885,-0.8693894762,0.6212629425\C,0
,1.1661978459,-2.3071311864,-1.8712281139\C,0,1.8977109461,-2.89533375
83,-3.098308837\C,0,2.668713231,-1.8067132862,-3.8558769017\C,0,2.7870
695384,-4.0786739495,-2.6956125826\O,0,0.9184473739,-3.397911858,-3.98
19134353\O,0,3.2385501897,2.8467006771,2.8479266994\O,0,-0.0539439933,
-2.3669493812,-1.866992685\H,0,5.1650240177,2.8129809973,3.484303179\H
,0,4.0528362227,1.8500322442,4.4806661492\H,0,5.4885209194,0.3565656565
9,3.0784781818\H,0,4.8634195174,1.1861957674,1.6139328703\H,0,3.518932
8896,-1.4073529245,-3.3009501436\H,0,1.9954917789,-0.9830342505,-4.109
0310403\H,0,3.0318070416,-2.2467633274,-4.7884250223\H,0,3.6433977158,
-3.7928788655,-2.0829282611\H,0,3.1515460278,-4.5461292173,-3.61419011
03\H,0,2.1953157031,-4.8188533499,-2.150016541\H,0,0.0522889175,-3.232
3274054,-3.5750581414\H,0,2.4553762686,2.2493680089,2.7863735409\H,0,-
0.3072246391,-0.3676995014,2.4027158933\N,0,0.7869769201,1.4400106401,
2.6152032094\H,0,1.0773424389,-0.4067627514,3.5168312158\H,0,-0.012471
0609,-1.2857966567,0.2240192578\C,0,0.1026964739,1.9169870983,3.812093
4028\C,0,0.2187862025,2.0549660457,1.4193927666\H,0,-0.9666632973,1.64
3050685,3.8146162383\H,0,0.1858384239,3.0053931557,3.8673856957\H,0,0.
5771984128,1.4895388396,4.6997975499\H,0,-0.8470239631,1.7952728418,1.
2923718923\H,0,0.7677521505,1.7267707724,0.5341015969\H,0,0.3107068601
,3.1412316704,1.4973296627\\Version=ES64L-G16RevA.03\State=1-A\HF=-940
.7294035\RMSD=2.298e-09\PG=C01 [X(C15H23N1O4)]\\@

Para-

1\1\GINC-R53\SP\RM062X TD-FC\6-31+G(d,p)\C14H21N1O3\ROOT\18-Apr-2019\0
\\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50)
guess=read geom=allcheck maxdisk=2147483648\\title\\0,1\C,-1.741131678
3,2.3393630911,-1.6774405458\C,-0.897788775,1.658468407,-0.6135716444\
O,0,1.433297562,0.9219136015,-1.2487510588\C,1.019538463,0.2461479911,-
0.4731102389\C,2.0165434758,-0.4645781025,-1.1546573353\H,2.0252410004
,-0.4313220915,-2.2386510402\C,2.9615310625,-1.1892856077,-0.449576906
9\H,3.7145343362,-1.7241905002,-1.0132174074\C,2.9414805785,-1.2294249
162,0.9550919636\C,1.9378077927,-0.5133268868,1.6177267731\H,1.9193527
49,-0.5415138676,2.7020462473\C,0.9819400911,0.2206820079,0.9260445127
\H,0.2237226881,0.7626315507,1.4774304426\C,3.9074518802,-1.9771587948
,1.8127813331\C,5.0792029011,-2.8088679003,1.245173618\C,4.5643232427,
-3.9802322046,0.3987924381\C,6.0696052173,-1.9189358338,0.4835364439\
O,5.7800308622,-3.3650338672,2.3369935446\N,-1.2152465871,3.6269860365,
-2.1042009309\O,3.7845754211,-1.9437496611,3.0279724515\H,-2.733718476
,2.516793144,-1.2496461826\H,-1.8669447722,1.6379125598,-2.5258916203\
H,-1.5163664035,0.9650474527,-0.02973781\H,-0.4715259991,2.4143163494,
0.0590337449\H,4.0817405984,-3.6698503086,-0.5291689172\H,3.8562489388
, -4.5757781068,0.9816462068\H,5.4210182786,-4.6142603142,0.1553491933\
H,5.6630407905,-1.5047834263,-0.4402874894\H,6.9441866171,-2.528616842
1,0.2414591722\H,6.3968300868,-1.0955204297,1.1243460075\H,5.326677693
8,-3.0748923963,3.1455064042\C,-2.1765356634,4.301769157,-2.9610986507
\C,0.0701019561,3.5092847409,-2.7793831152\H,-3.1227399289,4.432498325
4,-2.4285070524\H,-2.3757934262,3.7424352827,-3.8947096852\H,-1.795453
6288,5.2904251839,-3.2295181204\H,0.818141103,3.0843506416,-2.10853399
55\H,0.4039453335,4.5046696775,-3.0836442587\H,0.0111714237,2.86684685
78,-3.6778484909\\Version=ES64L-G16RevA.03\State=1-A\HF=-826.2259272\R

MSD=2.948e-09\PG=C01 [X(C14H21N1O3)]\@

I2959- NMe₂ Toluene

Ortho-

```
1\1\GINC-R208\SP\RM062X TD-FC\6-31+G(d,p)\C15H23N1O4\ROOT\25-Jan-2019\
0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=tol
uene) td(nstates=10,50-50) maxdisk=2684354560\title\0,1\C,0,-1.58325
08651,2.1664404674,-2.6741490329\C,0,-1.7215451783,3.6229655251,-3.058
1779387\O,0,-2.7100266366,4.1691023959,-2.1908254438\C,0,-3.0862828657
,5.461653436,-2.3704685966\C,0,-4.0922713383,5.9299975219,-1.513804801
\C,0,-4.5483541843,7.2353557896,-1.5993800584\C,0,-5.6484018036,7.7401
778349,-0.6920130923\C,0,-4.0105840241,8.0972852528,-2.5790610487\C,0,
-3.0222519284,7.6184480782,-3.4325196181\H,0,-2.5828535746,8.268478208
8,-4.1815286051\C,0,-2.5437092371,6.3087711182,-3.3340934997\H,0,-1.76
26650437,5.9748355402,-4.0061196723\C,0,-4.478786358,9.5243206755,-2.6
210111422\C,0,-5.053289073,10.1537512486,-3.9075516215\C,0,-3.89361940
22,10.6912387796,-4.7631101499\C,0,-5.9225900642,9.1900067951,-4.70134
96619\O,0,-5.8664218865,11.2463431677,-3.5180238488\O,0,-2.7896512017,
1.4588799363,-2.8776498632\O,0,-4.3699235394,10.2348786853,-1.63570357
86\H,0,-1.2534750285,2.0927963178,-1.6287107833\H,0,-0.8261886523,1.69
67746308,-3.3074839552\H,0,-2.0530187071,3.7110459095,-4.1005941886\H,
0,-0.7677132436,4.1508804808,-2.9290465145\H,0,-3.3032656968,9.8953186
97,-5.2231827939\H,0,-3.2335621499,11.3284466613,-4.1661297041\H,0,-4.
3270800005,11.2980331105,-5.5633332852\H,0,-5.3470276112,8.3305542958,
-5.0556509634\H,0,-6.3319741906,9.7179663668,-5.5679874903\H,0,-6.7473
27235,8.8367647314,-4.0793888601\H,0,-5.5427200808,11.5406497323,-2.65
21125395\H,0,-3.4779688107,1.8998188214,-2.3626667593\H,0,-6.007827132
2,6.9202829031,-0.0451964731\N,0,-6.7269451815,8.3229952833,-1.4825657
007\H,0,-5.2427090732,8.5207406628,-0.0420811451\C,0,-7.5088779137,9.2
79590386,-0.7198595615\C,0,-7.5644746241,7.292653077,-2.0730586868\H,0
,-8.0147428792,8.8208657266,0.1496180124\H,0,-8.2703326008,9.723496324
8,-1.3677088415\H,0,-6.8536783469,10.0794006204,-0.361586416\H,0,-8.07
84864046,6.6833836383,-1.3066733935\H,0,-6.9570877942,6.6247125202,-2.
6925269955\H,0,-8.3254470381,7.7535679722,-2.7097799216\H,0,-4.5129563
997,5.2457686728,-0.7820207661\Version=ES64L-G16RevA.03\State=1-A\HF=
-940.7399228\RMSD=3.405e-09\PG=C01 [X(C15H23N1O4)]\@
```

Meta-

```
1\1\GINC-R224\SP\RM062X TD-FC\6-31+G(d,p)\C15H23N1O4\ROOT\25-Jan-2019\
0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=tol
uene) td(nstates=10,50-50) maxdisk=2684354560\title\0,1\C,0,0.760972
5817,-3.6636431131,3.0296799768\C,0,1.3089352219,-3.515151345,1.623775
4055\O,0,0.6966588964,-2.3348920511,1.0899937612\C,0,1.4593445436,-1.3
892893659,0.5003693448\C,0,1.051166693,-0.0571303784,0.6889422133\C,0,
1.7751721315,0.9561285056,0.0737819564\C,0,-0.1256477503,0.2361456076,
1.5846331488\C,0,2.8988390936,0.683549033,-0.7218652644\C,0,3.28018136
49,-0.6549562523,-0.8908691307\H,0,4.1428961816,-0.8761043209,-1.51015
23424\C,0,2.5730733981,-1.6866224114,-0.2907295903\H,0,2.8718482392,-2
.718081781,-0.4452120439\C,0,3.7339782042,1.7137832057,-1.4041104709\C
,0,3.5046877575,3.2349159062,-1.249363785\C,0,2.1612718506,3.651022916
7,-1.8610041446\C,0,3.6509154651,3.677073599,0.2106362758\O,0,4.520051
3874,3.8946323819,-1.9817954601\O,0,1.1336862324,-2.5729931821,3.83266
98643\O,0,4.6579546119,1.3611582603,-2.1239437079\H,0,1.1689599228,-4.
5740265743,3.4818761239\H,0,-0.3334309975,-3.7723852552,2.9778794735\H
,0,1.0569559504,-4.3737909298,0.9912215608\H,0,2.3956190094,-3.3880110
588,1.6626840958\H,0,1.2962577564,3.2742953446,-1.3127178477\H,0,2.097
4583612,3.3045442273,-2.8968789548\H,0,2.1205405361,4.7440820094,-1.86
49871833\H,0,2.8458610216,3.3209152239,0.8558864529\H,0,3.6524334072,4
.7706740564,0.2298161185\H,0,4.6057756191,3.3287374494,0.6155619677\H,
0,5.0439724235,3.2055522888,-2.4227886956\H,0,0.7804933926,-1.74250123
85,3.4296424914\H,0,-0.4279568255,1.2911519817,1.4556431638\N,0,0.1620
528174,-0.0424866191,2.9969524456\H,0,-0.9737489891,-0.3914040104,1.29
36604437\H,0,1.4434296149,1.973380909,0.244329925\C,0,-1.0637680695,0.
0428886875,3.7838719215\C,0,1.1755687534,0.8636500353,3.5268890323\H,0
```

, -1.5167189692, 1.0485730214, 3.7381922594\H, 0, -0.8436844544, -0.19164163
47, 4.828762827\H, 0, -1.7900975758, -0.6857786634, 3.4121891006\H, 0, 0.8529
726576, 1.9188370206, 3.4691680404\H, 0, 2.1097270168, 0.7510848617, 2.97088
05964\H, 0, 1.3703035164, 0.6157646522, 4.5736746344\Version=ES64L-G16Rev
A.03\State=1-A\HF=-940.7493487\RMSD=6.267e-09\PG=C01 [X(C15H23N1O4)]\@

Para-

1\1\GINC-R58\SP\RM062X TD-FC\6-31+G(d,p)\C14H21N1O3\ROOT\18-Apr-2019\0
\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50)
scrf(smd,solvent=toluene) guess=read geom=allcheck maxdisk=2147483648\
\title\0,1\C,-1.4370445351,2.5620020429,-2.8096407156\C,-1.1596115329
,2.9579843211,-4.2485711816\O,-2.1710234559,3.865737397,-4.6861497261\
C,-2.114914406,4.3290971796,-5.9518403422\C,-1.1323645909,3.9710761917
, -6.8802888528\H,-0.3414044382,3.2784979402,-6.6209857109\C,-1.1698015
029,4.5121375074,-8.1638358853\H,-0.39157949,4.211683646,-8.8530968305
\C,-2.1702496533,5.4097458814,-8.5490347678\C,-3.1488000068,5.75609426
87,-7.5968469634\H,-3.9292440133,6.4519784287,-7.8852435524\C,-3.12755
85363,5.2291477189,-6.3216384643\H,-3.8806856597,5.4953585664,-5.58726
58465\C,-2.2898325752,6.0367811024,-9.8955531161\C,-1.3249874208,5.737
3324886,-11.0660874732\C,0.0997685052,6.2001094191,-10.7404373024\C,-1
.3873100928,4.2605375731,-11.4709209195\O,-1.7622149824,6.4914840299,-
12.1809583868\N,-2.354878822,1.4388553261,-2.6756172939\O,-3.194439667
9,6.8319997752,-10.1114222822\H,-1.7940872327,3.4556917927,-2.26135709
61\H,-0.4845000004,2.261962543,-2.3604651242\H,-1.1521815284,2.0646265
181,-4.8863693329\H,-0.1845960887,3.4562565073,-4.3180140676\H,0.57883
60402,5.6144001135,-9.9542819468\H,0.0933331102,7.2519767589,-10.43935
39982\H,0.6967571128,6.1110431719,-11.6526554703\H,-0.9738427865,3.586
2184977,-10.7192346193\H,-0.81558853,4.1425835275,-12.3959490184\H,-2.
4227588339,3.9694406078,-11.671354681\H,-2.5380907694,6.9995045902,-11
.8912286031\C,-3.6895206454,1.7458764201,-3.1714891897\C,-2.4189351093
,1.0099150169,-1.2874492609\H,-3.6609467363,1.9746691217,-4.2384839126
\H,-4.1419231971,2.6083183035,-2.647351086\H,-4.3335142669,0.874293030
2,-3.0252543613\H,-1.4204840624,0.7339225455,-0.9355768867\H,-3.066043
8737,0.1324311789,-1.2045124276\H,-2.8176687251,1.7972049501,-0.620427
3036\Version=ES64L-G16RevA.03\State=1-A\HF=-826.2442388\RMSD=6.382e-0
9\PG=C01 [X(C14H21N1O3)]\@

I2959- NMe₂ DCM

Ortho-

1\1\GINC-R64\SP\RM062X TD-FC\6-31+G(d,p)\C15H23N1O4\ROOT\21-Jan-2019\0
\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=dich
loromethane) td(nstates=10,50-50) maxdisk=2684354560\title\0,1\C,0,0
.4510780454,9.669229051,-4.1980233269\C,0,0,-0.4813308851,8.4807845054,-
4.1426781541\O,0,-1.5590775957,8.858581126,-3.2875526989\C,0,-2.510638
981,7.9346425795,-2.9997613394\C,0,-3.5182930219,8.349215873,-2.116504
1154\C,0,-4.538129777,7.4873834006,-1.7437503731\C,0,-5.6365521533,7.9
454894933,-0.809687313\C,0,-4.575055366,6.1823189475,-2.2815306665\C,0
, -3.5809267882,5.787619989,-3.1726904205\H,0,-3.5821677181,4.785347873
8,-3.5870493535\C,0,-2.54023246,6.6476399531,-3.5345884229\H,0,-1.7791
374051,6.3025741044,-4.2240468757\C,0,-5.6430664082,5.2358675096,-1.81
46521019\C,0,-6.584543581,4.5138438897,-2.8012472346\C,0,-7.0193784676
,5.3990020314,-3.9595338946\C,0,-5.9010074567,3.2323160285,-3.30588909
81\O,0,-7.7506050775,4.1459311931,-2.0805862074\O,0,0.9952730134,9.968
2310664,-2.9241943371\O,0,-5.7558209194,4.9804922353,-0.6261297802\H,0
, -0.0816333052,10.5367342562,-4.6098966414\H,0,1.2905875438,9.43406746
13,-4.8570924378\H,0,0.0355420674,7.6086042065,-3.7232138652\H,0,-0.85
7029564,8.2388018836,-5.144725245\H,0,-6.1641733143,5.7025094056,-4.56
93881814\H,0,-7.5235623324,6.2904932985,-3.5802148054\H,0,-7.714179639
2,4.8361836255,-4.5907353935\H,0,-5.0784084314,3.437113454,-3.99466136
59\H,0,-6.6542768768,2.6467414746,-3.8413809331\H,0,-5.5274926704,2.63
51775226,-2.4678057482\H,0,-7.4905963907,4.048470603,-1.1500169338\H,0
,0.2605581196,10.1548734507,-2.3227952436\H,0,-5.5811717345,7.37122911
38,0.1197122954\N,0,-6.9468460743,7.7111847164,-1.408691486\H,0,-5.487

6600122,9.0093236642,-0.5539629305\C,0,-7.2333511574,8.6948099681,-2.4
41763088\C,0,-7.9965642874,7.6799169721,-0.4039690801\H,0,-7.275583287
5,9.7219658138,-2.0352204607\H,0,-8.1965129334,8.4702378958,-2.9094396
318\H,0,-6.4597356709,8.6638195181,-3.2158806194\H,0,-8.084399763,8.63
38584484,0.1476435823\H,0,-7.7906920122,6.8801807445,0.3143693039\H,0,
-8.9562221364,7.4732889834,-0.8871670337\H,0,-3.4898661341,9.365288668
8,-1.7317443432\\Version=ES64L-G16RevA.03\State=1-A\HF=-940.7467222\RM
SD=6.613e-09\PG=C01 [X(C15H23N1O4)]\@

Meta-

1\1\GINC-R68\SP\RM062X TD-FC\6-31+G(d,p)\C15H23N1O4\ROOT\21-Jan-2019\0
\\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=dich
loromethane) td(nstates=10,50-50) maxdisk=2684354560\\title\\0,1\C,0,4
.2280563787,2.2094813681,3.2798838806\C,0,4.6157085119,0.9564000311,2.
5209593566\O,0,3.4854733664,0.0773135059,2.613755405\C,0,2.9585805481,
-0.4659344684,1.4951923725\C,0,1.5610222155,-0.6230999716,1.4811177491
\C,0,0.9659752813,-1.2154314441,0.3742255334\C,0,0.7458892862,-0.10825
0278,2.6403793831\C,0,1.7230977148,-1.6535679326,-0.7243168251\C,0,3.1
150241901,-1.4829491372,-0.6797603382\H,0,3.7118926203,-1.8237407998,-
1.5191548596\C,0,3.7351623708,-0.8975252782,0.414637258\H,0,4.81445907
78,-0.7884408135,0.4396503284\C,0,1.1605382617,-2.2876413503,-1.949620
0956\C,0,-0.3546647081,-2.4554598636,-2.2035335617\C,0,-0.9686712772,-
3.4396347216,-1.2008353078\C,0,-1.0755177588,-1.1041378332,-2.22193235
32\O,0,-0.5076246065,-3.0197404869,-3.4963959357\O,0,3.120647573,2.841
1245487,2.6787045902\O,0,1.9187480714,-2.7020433607,-2.8180865277\H,0,
5.0687161644,2.9112190431,3.2697915471\H,0,4.0172379027,1.9456343459,4
.3272415861\H,0,5.4908048959,0.4664374315,2.9606074425\H,0,4.816018945
1,1.2015570896,1.4734522092\H,0,-0.9864527294,-3.0604977177,-0.1779060
349\H,0,-0.4161224137,-4.3841756132,-1.2165990257\H,0,-1.9982396382,-3
.6373589482,-1.51379491\H,0,-1.1309876017,-0.6318102865,-1.2397883178\
H,0,-2.0951995898,-1.274291677,-2.5800356148\H,0,-0.5767019613,-0.4197
182868,-2.914971422\H,0,0.3844607413,-3.2170483792,-3.8290743939\H,0,2
.3462522553,2.2210215898,2.7004174823\H,0,-0.2849730755,-0.4952367723,
2.5615574257\N,0,0.7339843745,1.3598886159,2.7055428881\H,0,1.17048772
14,-0.4746023738,3.5801255626\H,0,-0.1127971984,-1.3141669099,0.390836
7867\C,0,0.1387989955,1.797209259,3.9657870516\C,0,0.0113976537,1.9367
557943,1.5748025223\H,0,-0.903822665,1.4517240891,4.0706581176\H,0,0.1
490500481,2.889620973,4.0134087199\H,0,0.7242098818,1.4059754427,4.803
0417471\H,0,-1.0405908252,1.6024799504,1.5496142231\H,0,0.4921679813,1
.6526801992,0.6349536308\H,0,0.0292470201,3.027253427,1.6533877242\\ve
rsion=ES64L-G16RevA.03\State=1-A\HF=-940.7555532\RMSD=5.451e-09\PG=C01
[X(C15H23N1O4)]\@

Para-

1\1\GINC-R62\SP\RM062X TD-FC\6-31+G(d,p)\C14H21N1O3\ROOT\18-Apr-2019\0
\\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50)
scrf(smd,solvent=dichloromethane) guess=geom=allcheck maxdisk=214
7483648\\title\\0,1\C,-1.1325446834,2.209001779,-2.6357752047\C,0.0347
497812,1.3145505171,-2.262396405\O,0.0867292846,1.187695688,-0.8379235
985\C,1.0491013043,0.4147072213,-0.2962516642\C,2.0089932624,-0.284536
3957,-1.0360875934\H,2.025896215,-0.2392745722,-2.1179742236\C,2.96235
57109,-1.0539950048,-0.37229134\H,3.688039194,-1.5764371579,-0.9817536
821\C,2.9846993561,-1.1442601004,1.024128022\C,2.0078545454,-0.4315663
206,1.7481856056\H,2.0121105498,-0.4923107407,2.8313459861\C,1.0549324
91,0.3338452635,1.1067343276\H,0.3024965682,0.8815812332,1.6652547577\
C,3.9656418025,-1.9355806569,1.8159209928\C,5.0614342347,-2.8213951305
,1.1807551116\C,4.4515582218,-3.9369356905,0.3267034249\C,6.074260869,
-1.9708157011,0.406160153\O,5.7651774626,-3.4495484217,2.240828933\N,-
2.4047100055,1.5051128551,-2.7602220548\O,3.9214448098,-1.900592738,3.
0402045699\H,-0.907862958,2.6561244389,-3.6094473827\H,-1.1935738352,3
.0339135654,-1.8997102109\H,0.9736282019,1.7612445338,-2.6101036803\H,
-0.0822592029,0.3251261578,-2.722137561\H,3.9752960488,-3.5698592625,-
0.5835906419\H,3.7135884594,-4.4962597167,0.9099320238\H,5.2574395789,
-4.6207192788,0.0437602282\H,5.6578973147,-1.5163759515,-0.4940645126\
H,6.9030052964,-2.6221187544,0.112875994\H,6.4694472578,-1.1789749502,

1.0500303651\H,5.3892984646,-3.1107786224,3.0712078267\C,-3.4235231705
,2.418481294,-3.2597868313\C,-2.8375099072,0.9172299096,-1.498116087\H
,-3.114108077,2.8307515904,-4.2247063052\H,-3.6071971697,3.2590521689,
-2.5652995474\H,-4.3641462193,1.8785121449,-3.3994185258\H,-2.12519425
71,0.1611767032,-1.1613694348\H,-3.8083988844,0.4350995994,-1.64281346
59\H,-2.9390779152,1.6758985042,-0.7001483689\Version=ES64L-G16RevA.0
3\State=1-A\HF=-826.2505114\RMSD=1.833e-09\PG=C01 [X(C14H21N1O3)]\@

I2959- NMe₂ Acetonitrile

Ortho-

1\1\GINC-R3204\SP\RM062X TD-FC\6-31+G(d,p)\C15H23N1O4\ROOT\05-Jan-2019
\0\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=ac
etonitrile) td(nstates=10,50-50) maxdisk=2684354560\title\0,1\C,0,-1
.754035856,2.2995374929,-2.7877442792\C,0,-0.600410299,1.3732207116,-2
.4803305857\O,0,-0.5232584685,1.2871051366,-1.057215316\C,0,0.39553995
35,0.4520322894,-0.5105744535\C,0,0.3938099563,0.3722021003,0.88994781
33\C,0,1.2832558659,-0.4551884317,1.5586272987\C,0,1.2917982067,-0.513
1090719,3.0701250931\C,0,2.2204393088,-1.2085721978,0.8180800581\C,0,2
.226884964,-1.1062909712,-0.570891908\H,0,2.9294210244,-1.6849764404,-
1.1604874114\C,0,1.3178051731,-0.2891871675,-1.2484801482\H,0,1.347742
4851,-0.2425355596,-2.3304909157\C,0,3.1313401947,-2.1546120763,1.5451
613083\C,0,4.6651485484,-2.096800292,1.3847216022\C,0,5.0771184754,-2.
9122375619,0.1484464717\C,0,5.1967233478,-0.6735224302,1.3069216126\O,
0,5.2336604089,-2.7076920313,2.5340330858\O,0,-2.9863937155,1.77822144
34,-2.3173655778\O,0,2.6629585014,-3.0313228289,2.2544301629\H,0,-1.84
44681945,2.4072826186,-3.8714281259\H,0,-1.5580219096,3.2895887268,-2.
3552464785\H,0,0.3345850175,1.7756377883,-2.8888772336\H,0,-0.78577098
26,0.3772113075,-2.9012472213\H,0,4.800112044,-2.4248396861,-0.7886914
244\H,0,4.6335860263,-3.9127282044,0.1773787135\H,0,6.1664236013,-3.01
3185907,0.1694674445\H,0,4.8138881593,-0.1572181718,0.4224701472\H,0,6
.2887297947,-0.7090360119,1.2417477959\H,0,4.9098128185,-0.114736425,2
.2007850413\H,0,4.5797983104,-3.3431482115,2.8684345212\H,0,-2.9118480
323,1.6621712173,-1.3602211658\H,0,0.541526614,0.1906028769,3.47149195
22\N,0,2.6271617192,-0.2299073271,3.5878036757\H,0,1.0099328295,-1.518
8646551,3.3951989063\C,0,2.7701215086,-0.6929740086,4.9585260203\C,0,2
.9399764647,1.1875098638,3.4791608152\H,0,2.0608935917,-0.1990915022,5
.6476271627\H,0,3.7863746014,-0.4878300075,5.3084134713\H,0,2.59906562
25,-1.7732434451,4.9997430573\H,0,2.2480953803,1.8100283796,4.07549495
38\H,0,2.8768745946,1.508789623,2.4344842821\H,0,3.9591834133,1.368360
0585,3.8332463481\H,0,-0.3154300681,0.9783619894,1.4475944298\Version
=ES64L-G16RevA.03\State=1-A\HF=-940.7465058\RMSD=6.283e-09\PG=C01 [X(C
15H23N1O4)]\@

Meta-

1\1\GINC-R3453\SP\RM062X TD-FC\6-31+G(d,p)\C15H23N1O4\ROOT\05-Jan-2019
\0\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=ac
etonitrile) td(nstates=10,50-50) maxdisk=2684354560\title\0,1\C,0,2.
2153117268,-5.1205423595,-0.98425697\C,0,2.3173338678,-4.4007037682,0.
3449235869\O,0,3.1730760171,-3.2712604289,0.114757466\C,0,2.7628878136
, -2.0325397166,0.4615676227\C,0,3.1596650918,-0.9839010755,-0.39230163
99\C,0,2.8082834164,0.31222342,-0.0508198797\C,0,3.9167811251,-1.30329
86099,-1.6564179388\C,0,2.063934959,0.6058277668,1.106902465\C,0,1.675
0836362,-0.4583373641,1.9314203107\H,0,1.110674652,-0.2957557747,2.840
4091753\C,0,2.0245620588,-1.7680463807,1.6173578856\H,0,1.7386310102,-
2.5783682653,2.2795642567\C,0,1.7485667623,2.040208019,1.3554942005\C,
0,0.8333241039,2.5251054826,2.5018796648\C,0,-0.5678892684,1.917648627
,2.4009644788\C,0,1.4924953964,2.268600543,3.8621758575\O,0,0.68407900
07,3.9297443325,2.3584058959\O,0,1.6174400462,-4.2969271487,-1.9605775
823\O,0,2.2261799315,2.9002850231,0.624423641\H,0,1.5937818899,-6.0137
410736,-0.8618117369\H,0,3.2192802343,-5.4446767823,-1.2968229562\H,0,
2.7588915152,-5.0354261307,1.1199878971\H,0,1.3268214819,-4.0626767094
,0.6643269182\H,0,-0.587588936,0.8489066151,2.6182712474\H,0,-0.979571
0021,2.0822918274,1.4003804262\H,0,-1.2077162715,2.428622731,3.1266789
178\H,0,1.5782001023,1.2082170979,4.1045446704\H,0,0.8781582378,2.7500

213858,4.628961343\H,0,2.4906234385,2.7171243605,3.8852190106\H,0,1.28
54129916,4.2062122628,1.6461274194\H,0,2.1897445193,-3.4967983764,-2.0
982907168\H,0,4.3140402442,-0.3692374212,-2.0886595755\N,0,3.085304629
7,-2.0077617574,-2.6432315025\H,0,4.7657457401,-1.95272351,-1.42132975
28\H,0,3.1011539265,1.128163009,-0.7058290362\C,0,3.9234596653,-2.5085
858784,-3.7298925672\C,0,2.0376952611,-1.1374764036,-3.1717444522\H,0,
4.449787608,-1.6920401348,-4.2525665092\H,0,3.3002103445,-3.0396215407
, -4.454792356\H,0,4.665855814,-3.2051185737,-3.3293373814\H,0,2.460483
6473,-0.2501414467,-3.6734921205\H,0,1.3818460445,-0.8030368693,-2.363
6265025\H,0,1.4365415263,-1.6951320034,-3.8954061807\\Version=ES64L-G1
6RevA.03\State=1-A\HF=-940.7552584\RMSD=5.668e-09\PG=C01 [X(C15H23N1O4
)]\@

Para-

1\1\GINC-R61\SP\RM062X TD-FC\6-31+G(d,p)\C14H21N1O3\ROOT\18-Apr-2019\
\\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50)
scrf(smd,solvent=acetonitrile) guess=read geom=allcheck maxdisk=214748
3648\\title\\0,1\C,-1.2054076022,2.0084956425,-2.8661609214\C,-0.01913
11074,1.1267847226,-2.5368932509\O,-0.1379823658,-0.0868770663,-3.2809
180002\C,0.8298344506,-1.0145628225,-3.1503328709\C,1.9577544206,-0.86
83131784,-2.3344335293\H,2.1177958463,0.0323024709,-1.7546495256\C,2.8
943836421,-1.8972932646,-2.2636122247\H,3.7526822031,-1.7420884915,-1.
622620098\C,2.7398250594,-3.0771402232,-3.0009523504\C,1.6022625401,-3
.1983626418,-3.8241481729\H,1.4677079691,-4.1064612214,-4.402533457\C,
0.6595553489,-2.1923306075,-3.8986122725\H,-0.2205130518,-2.2916812042
, -4.5261592707\C,3.6881908064,-4.2231707914,-2.9873608527\C,4.87011064
96,-4.3385298489,-1.9985466899\C,5.9485370539,-3.2987224667,-2.3271214
223\C,4.4030743606,-4.2622554795,-0.543545147\O,5.445600402,-5.6242135
997,-2.1770539772\N,-2.4958867412,1.4663279215,-2.4555111067\O,3.54026
10254,-5.14140542,-3.7861629818\H,-1.2287769904,2.162657735,-3.9503363
974\H,-1.0210031832,2.9940089989,-2.3955268051\H,0.0406013001,0.897396
9531,-1.4671413308\H,0.9004566812,1.6480822055,-2.829321355\H,5.626323
2232,-2.2721282611,-2.1460281143\H,6.2526333054,-3.3924890968,-3.37439
89191\H,6.8170292852,-3.5048299029,-1.6943142678\H,4.0661385463,-3.265
5984878,-0.2555674865\H,5.2485914707,-4.536599857,0.094448058\H,3.5913
697336,-4.9751043077,-0.3683278299\H,5.0335222086,-6.0100728866,-2.968
6293983\C,-3.5668956665,2.286760212,-3.006346255\C,-2.6195538086,1.402
5045232,-1.0049663551\H,-3.4973064742,2.3064439218,-4.097711761\H,-3.5
250265055,3.3282244848,-2.6363404634\H,-4.5359377066,1.8635481269,-2.7
274312178\H,-1.8851894567,0.7143079895,-0.579771479\H,-3.6149195908,1.
033108274,-0.7435634577\H,-2.4825202816,2.3944749454,-0.535171043\\Ver
sion=ES64L-G16RevA.03\State=1-A\HF=-826.2499562\RMSD=2.068e-09\PG=C01
[X(C14H21N1O3)]\@

I2959- NMe₂ Water

Ortho-

1\1\GINC-R59\SP\RM062X TD-FC\6-31+G(d,p)\C15H23N1O4\ROOT\25-Jan-2019\
\\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=h2o)
td(nstates=10,50-50) maxdisk=2684354560\\title\\0,1\C,0,2.3445225735,
-4.4820744952,-2.8167616074\C,0,2.0431378175,-3.0434555606,-2.47234216
65\O,0,1.904627123,-2.9748314226,-1.0514057373\C,0,1.6695054324,-1.758
168449,-0.4878378453\C,0,1.5861863537,-1.7405013747,0.9107714422\C,0,1
.3311238047,-0.5637184011,1.600421901\C,0,1.2980218946,-0.5829926115,3
.1120476504\C,0,1.1819664192,0.6372975462,0.8728252864\C,0,1.297431745
2,0.6129689494,-0.5165452773\H,0,1.1856308207,1.5267826937,-1.09014183
73\C,0,1.5251296149,-0.575241827,-1.21170562\H,0,1.5878030698,-0.55736
51826,-2.2927841151\C,0,0.8530814576,1.905137897,1.5932849915\C,0,1.68
21039658,3.1912427119,1.389695601\C,0,3.1498819465,2.9131470546,1.1059
562241\C,0,1.0361622201,4.0310566847,0.2809621817\O,0,1.6258470265,3.9
237797086,2.6115068241\O,0,3.6022729902,-4.9033159735,-2.3025519583\O,
0,-0.1057948618,1.9567989378,2.3520421068\H,0,2.3970284893,-4.57868856
16,-3.9034524375\H,0,1.5414173816,-5.1302447601,-2.4463988191\H,0,1.11
15611139,-2.7267077316,-2.9559683097\H,0,2.863535467,-2.3911574766,-2.
7939955673\H,0,3.276840684,2.4349315548,0.1324382435\H,0,3.5813770647,

2.2668795764,1.8759913715\H,0,3.6901244128,3.8642414173,1.0975281771\H,0,1.0907534217,3.5456070502,-0.6956546402\H,0,1.5722227743,4.9828893981,0.2221839517\H,0,-0.0129958848,4.229038789,0.520901293\H,0,0.7098863991,3.888573982,2.9311244207\H,0,3.5507123934,-4.9009942111,-1.3367214731\H,0,0.3135692936,-0.2682279828,3.4700544636\N,0,2.2976388883,0.3138635329,3.6958048186\H,0,1.4574494633,-1.6205943239,3.4549572057\C,0,3.6459684488,-0.1450767347,3.3779947214\C,0,2.1161706172,0.3498121676,5.1434026649\H,0,3.8309232966,-1.1666834444,3.7564404324\H,0,4.3777990636,0.528477536,3.8320912177\H,0,3.8053576237,-0.146070196,2.2961171874\H,0,2.2299388364,-0.6501253739,5.5982324625\H,0,1.1174119938,0.7266567188,5.382421866\H,0,2.8571978711,1.0167234581,5.5919526901\H,0,1.7352604728,-2.6698292706,1.4536530144\\Version=ES64L-G16RevA.03\State=1-A\HF=-940.7432073\RMSD=9.737e-09\PG=C01 [X(C15H23N1O4)]\\@

Meta-

1\1\GINC-R61\SP\RM062X TD-FC\6-31+G(d,p)\C15H23N1O4\ROOT\25-Jan-2019\0\\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=h2o) td(nstates=10,50-50) maxdisk=2684354560\\title\\0,1\C,0,-1.2215089548,1.7706116565,-2.718017472\C,0,-1.6074470387,3.1425780472,-3.2155835247\O,0,-2.3732417267,3.7664983069,-2.1800527526\C,0,-2.7971069761,5.0402986612,-2.3649640715\C,0,-3.5238409205,5.6242711633,-1.3078601244\C,0,-3.93604498,6.9454924146,-1.4427141221\C,0,-3.8920114039,4.8501756638,-0.0553275242\C,0,-3.6765817101,7.6973345702,-2.599066891\C,0,-2.9651376314,7.0818152209,-3.6376563419\H,0,-2.7577888837,7.6393549715,-4.5448381103\C,0,-2.5249232601,5.7710152136,-3.5301389956\H,0,-1.9759211342,5.327189971,-4.3511871098\C,0,-4.103011782,9.1045886073,-2.806374257\C,0,-5.1382434052,9.8131659778,-1.9080960555\C,0,-6.4236445296,9.0068825945,-1.7340669216\C,0,-4.4839434388,10.1824917252,-0.5711683747\O,0,-5.5166064729,11.0176321829,-2.568028387\O,0,-2.3529904426,0.9327733114,-2.5176248427\O,0,-3.6241526925,9.7579795438,-3.7305131439\H,0,-0.64102588,1.859334776,-1.7922132446\H,0,-0.5981240926,1.2898295723,-3.475324008\H,0,-2.2143373301,3.06847431,-4.1254394335\H,0,-0.7051092571,3.7295870629,-3.4210893775\H,0,-6.29324744,8.1385599458,-1.0872635821\H,0,-6.8006420888,8.6715812961,-2.7048636812\H,0,-7.1703570779,9.6624622827,-1.2765241976\H,0,-4.1740085373,9.310039292,0.0064767248\H,0,-5.2108439241,10.7491294781,0.0181407092\H,0,-3.6077473683,10.8131757718,-0.7497291948\H,0,-4.7828681586,11.2687613722,-3.1536113348\H,0,-2.853084742,1.2788309933,-1.7658260809\H,0,-3.1542735751,4.0659203401,0.1301898301\N,0,-5.2234654025,4.2193862237,-0.0648022313\H,0,-3.8660628286,5.5421051413,0.7920049882\H,0,-4.456242121,7.38105713,-0.5972001128\C,0,-5.3285696967,3.1959828795,-1.1000394036\C,0,-6.2923679837,5.1989611869,-0.2401024716\H,0,-5.2048733677,3.6014269723,-2.118684106\H,0,-6.3150461608,2.7281010816,-1.0436524358\H,0,-4.572786194,2.4242241818,-0.9365672396\H,0,-6.3016581175,5.65210763,-1.2450925233\H,0,-6.1909481313,5.9995065466,0.4987062045\H,0,-7.2565651407,4.7065427293,-0.0872607752\\Version=ES64L-G16RevA.03\State=1-A\HF=-940.7491696\RMSD=8.023e-09\PG=C01 [X(C15H23N1O4)]\\@

Para-

1\1\GINC-R54\SP\RM062X TD-FC\6-31+G(d,p)\C14H21N1O3\ROOT\18-Apr-2019\0\\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50) scrf(smd,solvent=h2o) guess=read geom=allcheck maxdisk=2147483648\\title\\0,1\C,-1.240358693,1.9745794503,-2.9015013117\C,-0.0432926102,1.1084134797,-2.5800036432\O,-0.1671880643,-0.1228821744,-3.299024866\C,0.8188547081,-1.0426472231,-3.1696155346\C,1.9597856193,-0.8621092484,-2.3815246233\H,2.119785502,0.0534829543,-1.8261269881\C,2.9109281322,-1.8769669998,-2.3098076086\H,3.7832473762,-1.6959371379,-1.6949198607\C,2.7572546271,-3.0706190822,-3.0251024269\C,1.6048976414,-3.2252758245,-3.8205643246\H,1.4661285198,-4.1452767064,-4.3783169442\C,0.6445956149,-2.2352844227,-3.8893990569\H,-0.2494037574,-2.3601179454,-4.4917330405\C,3.7328846211,-4.1908298171,-3.0239341803\C,4.8510733692,-4.3386808282,-1.9710138656\C,5.9773199035,-3.3427722588,-2.2745545744\C,4.3322589462,-4.2242792132,-0.5400029838\O,5.3759698403,-5.6572733911,-2.0938609162\N,-2.52956828,1.4398085116,-2.4614736483\O,3.6659075287,-5.0561151573,-3.8938320987\H,-1.2811176497,2.1204419907,-3.9857154212\H,-

1.0521061263,2.9639629823,-2.444098532\H,0.0418897891,0.8977580528,-1.5087422633\H,0.864840189,1.6287773169,-2.9047781153\H,5.6623986933,-2.3025259453,-2.1757890485\H,6.3496596908,-3.5017293863,-3.2911765678\H,6.7922700435,-3.5273713828,-1.568613994\H,4.0443721315,-3.2061372576,-0.2779533183\H,5.1352710893,-4.5353295989,0.1345898944\H,3.473836779,-4.8856209821,-0.3904801854\H,5.2242231611,-5.9463094829,-3.0090914991\C,-3.5796085948,2.3385294229,-2.9364028311\C,-2.5898713324,1.3784434772,-1.0025318595\H,-3.5559514952,2.3986811528,-4.0274687479\H,-3.4605175191,3.358419775,-2.5301788949\H,-4.5580904585,1.9604177173,-2.6307696936\H,-1.8774748311,0.6498860225,-0.6104935143\H,-3.5904298248,1.0658212398,-0.6946190656\H,-2.3764832797,2.3598659204,-0.5431478465\\Version=ES64L-G16RevA.03\State=1-A\HF=-826.2466062\RMSD=9.347e-10\PG=C01 [X(C14H21N1O3)]\@

I2959- NMe₂H Gas

Ortho-

1\1\GINC-R401\SP\RM062X TD-FC\6-31+G(d,p)\C15H24N1O4(1+)\ROOT\21-Jan-2019\0\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50) maxdisk=2684354560\\title\\1,1\C,0,-0.1670170135,9.0050803179,-4.5631788257\C,0,-1.5099644844,8.3449449333,-4.3290240687\O,0,-1.9099316607,8.6988515649,-2.9979816526\C,0,-3.026498535,8.1618411841,-2.4902903973\C,0,-3.325758667,8.5160350054,-1.1619837988\C,0,-4.4566987942,8.0300827146,-0.5290249815\C,0,-4.6874628549,8.4679730118,0.8973530501\C,0,-5.3219900954,7.1321620847,-1.2126341508\C,0,-5.0000280295,6.7834770498,-2.5299170735\H,0,-5.642056804,6.0976138788,-3.0661673988\C,0,-3.8825987103,7.2989549948,-3.1776120333\H,0,-3.6847857699,7.0116643824,-4.20245723\C,0,-6.572270171,6.649207205,-0.5749739298\C,0,-7.1896761856,5.267723301,-0.8293981346\C,0,-7.3059287308,4.567550667,0.53045602\C,0,-8.5396465406,6.1444324196,-2.8314357062\O,0,-6.3256770124,4.536187763,-1.679809782\O,0,0.8198845561,8.4829622272,-3.7070166447\O,0,-7.1709645165,7.3630165584,0.235689265\H,0,-0.267613295,10.093102903,-4.4540061256\H,0,-0.1547940975,8.7932003715,-5.5857715644\H,0,-1.4084224296,7.2558890242,-4.3968557826\H,0,-2.2602089311,8.7022197593,-5.045148049\H,0,-7.9405443764,5.1386880839,1.2095275754\H,0,-6.3171804317,4.4327558587,0.9785968354\H,0,-7.7551119609,3.5798905662,0.3850530228\H,0,-6.6214639078,8.9140455805,0.5920812254\H,0,-9.5455055305,6.2229082581,-3.2490603839\H,0,-8.1349950398,7.1610902034,-2.7609726422\H,0,-6.6061137758,3.6127473306,-1.6932005874\H,0,0.6266772363,8.75620808,-2.8030820622\H,0,-4.9885730307,7.6419630866,1.5462231821\N,0,-5.80879814,9.4678212401,0.9636482843\H,0,-3.7941452104,8.9406694373,1.3102701685\C,0,-6.0986784622,9.9714042755,2.3340158536\C,0,-8.5782064143,5.4598807544,-1.4684321113\H,0,-6.3836511949,9.1214952131,2.9539657353\H,0,-6.9204181875,10.6845212967,2.284141007\H,0,-5.2068265167,10.4499645689,2.7386643549\H,0,-9.0296299269,4.4643435335,-1.5602639796\H,0,-9.1967832233,6.0290052099,-0.7673917377\H,0,-7.926222947,5.579247276,-3.5383013824\H,0,-2.6295256889,9.1705636658,-0.6454393386\H,0,-5.6126053453,10.2415401592,0.3235619754\\Version=ES64L-G16RevA.03\State=1-A\HF=-941.1159063\RMSD=3.700e-09\PG=C01 [X(C15H24N1O4)]\@

Meta-

1\1\GINC-R402\SP\RM062X TD-FC\6-31+G(d,p)\C15H24N1O4(1+)\ROOT\21-Jan-2019\0\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50) maxdisk=2684354560\\title\\1,1\C,0,0.242147083,-6.1421277889,-1.1864111396\C,0,1.1648790723,-4.953106955,-1.0518736856\O,0,0.640069098,-3.9608113869,-1.9323803187\C,0,1.458981601,-2.9702158821,-2.3834163982\C,0,1.0733989492,-2.4042586013,-3.6109147704\C,0,1.8465421668,-1.3933729641,-4.1586272468\C,0,-0.164752221,-2.9158836622,-4.2887769278\C,0,2.9942581681,-0.9192400277,-3.5063891792\C,0,3.3561785889,-1.5000454262,-2.2893970383\H,0,4.2392833159,-1.1700226149,-1.757786843\C,0,2.6008861181,-2.5299926108,-1.7257104387\H,0,2.8998917821,-2.9649616205,-0.778722951\C,0,3.7487047039,0.1751750187,-4.2160464899\C,0,4.8714226225,0.9935682571,-3.5564668685\C,0,4.4267078667,1.6188040898,-2.2311822719\C,0,6.1276097754,0.1189642438,-3.4054208367\O,0,5.185106366,2.0663855491,-4.4121449778\O,0,0.1988631474,-6.4786508814,-2.5766307016\O,0,3.

4521207992,0.4189698104,-5.3713244945\H,0,-0.7617554261,-5.8859193535,
-0.8304076584\H,0,0.6349722119,-6.9733741756,-0.5931281851\H,0,2.18073
54664,-5.2182355385,-1.3677922921\H,0,1.17935651,-4.5877097042,-0.0194
766906\H,0,4.2929592654,0.8903501024,-1.429999032\H,0,3.495775864,2.17
53057319,-2.3678859988\H,0,5.2011745156,2.3275858345,-1.9286332512\H,0
,6.002915581,-0.7146665246,-2.710580392\H,0,6.9330484844,0.7600146427,
-3.0390931685\H,0,6.4257905749,-0.2767143724,-4.3803609198\H,0,4.82060
18384,1.878732731,-5.2903663201\H,0,-0.1429569954,-7.3739023307,-2.682
1945381\H,0,-1.0466912312,-2.8034130701,-3.6519356309\N,0,-0.076281571
, -4.391155387,-4.6084286118\H,0,-0.3379155791,-2.3961221576,-5.2349560
518\H,0,1.5795876502,-0.9459227274,-5.1124041534\C,0,1.0927708144,-4.7
190516752,-5.4727988675\C,0,-1.3481913159,-4.8805364848,-5.2081582469\
H,0,0.0503249526,-4.898463521,-3.7130383124\H,0,0.9815092048,-4.195902
1133,-6.4246952521\H,0,1.1130028777,-5.7969465354,-5.6319870573\H,0,2.
0056617575,-4.3963797239,-4.9739703914\H,0,-1.5091268484,-4.3719047201
, -6.1601822967\H,0,-2.1681663464,-4.6653535213,-4.5230103725\H,0,-1.26
98392595,-5.9557149527,-5.3681837301\\Version=ES64L-G16RevA.03\State=1
-A\HF=-941.1187086\RMSD=2.982e-09\PG=C01 [X(C15H24N104)]\@

Para-

1\1\GINC-R82\SP\RM062X TD-FC\6-31+G(d,p)\C14H22N1O3(1+)\ROOT\18-Apr-20
19\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-
50) guess=read geom=allcheck maxdisk=2147483648\\title\\1,1\C,-1.86658
33508,2.381506582,-1.4689460248\C,-0.9895228721,1.621050693,-0.4872405
11\O,-0.4327291968,2.6126331787,0.3478052837\C,0.3924202503,2.21063170
54,1.3828980269\C,0.8933537203,3.230302049,2.1882204427\H,0.6147758845
,4.2588236527,1.984890928\C,1.733357555,2.9152098986,3.2477492044\H,2.
1085626772,3.7250030377,3.8591711665\C,2.0871047393,1.5850871493,3.511
4564782\C,1.5699181965,0.582815933,2.6860628978\H,1.8453698531,-0.4460
446424,2.8917551849\C,0.7210262391,0.879108079,1.6237355459\H,0.334041
5009,0.0710530274,1.0138194284\C,2.9960579228,1.1271546706,4.622441353
2\C,3.527865285,2.0643089889,5.7218019674\C,4.5244413359,3.0697970672,
5.1232890621\C,2.3873343478,2.7463390149,6.485729972\O,4.2254721161,1.
2796394144,6.6600991744\N,-1.1329290187,3.5871421238,-1.9901753228\O,3
.3283874761,-0.0432894653,4.6518363489\H,-2.7606384202,2.7586443909,-0
.967574467\H,-2.1588240128,1.766518097,-2.3236382801\H,-0.2031238976,1
.0490715562,-0.9962048891\H,-1.6151010181,0.9197575822,0.0770881801\H,
4.0695417319,3.7831865248,4.4329536425\H,5.3244819259,2.5360323525,4.6
029493585\H,4.9710284501,3.6233582334,5.9528758587\H,1.8454150827,3.48
58444915,5.8939473366\H,2.8275759225,3.2482691119,7.3507457807\H,1.680
8605939,1.9977370411,6.8540614509\H,4.3221280691,0.3847447035,6.299108
8507\C,-2.0363738331,4.4745615778,-2.7831531218\C,0.0974143426,3.22686
39071,-2.7609524679\H,-2.894563561,4.7477608277,-2.1697349728\H,-2.364
8479794,3.9285846327,-3.6686346851\H,-1.4853407119,5.3672566155,-3.077
664528\H,0.797628638,2.7205590304,-2.0980871443\H,0.5488235489,4.14237
46653,-3.1421126267\H,-0.1912575303,2.577941455,-3.5892356677\H,-0.821
9260027,4.0868090456,-1.1463592152\\Version=ES64L-G16RevA.03\State=1-A
\HF=-826.6008797\RMSD=2.376e-09\PG=C01 [X(C14H22N1O3)]\@

I2959- NMe₂H Toluene

Ortho-

1\1\GINC-R388\SP\RM062X TD-FC\6-31+G(d,p)\C15H24N1O4(1+)\ROOT\21-Jan-2
019\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent
=toluene) td(nstates=10,50-50) maxdisk=2684354560\\title\\1,1\C,0,-1.5
089273895,1.858419857,-2.6909891974\C,0,-0.355267987,1.0025174958,-2.2
179438042\O,0,-0.312723443,1.1401631716,-0.7929914466\C,0,0.5882542979
,0.4221222704,-0.0993826367\C,0,0.5491320797,0.5712202771,1.295426313\
C,0,1.4398384241,-0.1011229786,2.1179800153\C,0,1.2775717694,0.1006220
333,3.6054840676\C,0,2.3990445231,-0.9788307373,1.5463548626\C,0,2.406
0800928,-1.132030171,0.1538629349\H,0,3.1306991456,-1.7978058903,-0.29
90132071\C,0,1.5284972096,-0.4367537255,-0.6715724715\H,0,1.5842694106
, -0.577126286,-1.7440648817\C,0,3.3666846006,-1.7149855056,2.411101413
8\C,0,3.9135851006,-3.1024984119,1.9929221814\C,0,4.8303820116,-3.6542
562559,3.0756920058\C,0,2.7489824774,-4.0527605261,1.7291879434\O,0,4.

6277566816,-2.9611624075,0.7649218655\O,0,-2.7425055855,1.3962316048,-
2.1831078728\O,0,3.711577835,-1.2405024243,3.4894639176\H,0,-1.5703108
841,1.7998008657,-3.7804883799\H,0,-1.3296381997,2.9057226027,-2.41256
38916\H,0,0.5915764817,1.3443002339,-2.6540831792\H,0,-0.5296253395,-0
.0484383104,-2.4772237758\H,0,4.288836564,-3.8124266337,4.0110037195\H
,0,5.6591351357,-2.9705399615,3.282755227\H,0,5.2311711199,-4.61266453
34,2.735323678\H,0,2.1049271836,-4.1202501499,2.6120570209\H,0,3.14546
57399,-5.0474293653,1.5094272622\H,0,2.1449428124,-3.7230071274,0.8814
445876\H,0,5.5293035059,-2.6684142214,0.9549678293\H,0,-2.7168691821,1
.4640292175,-1.220410603\H,0,0.3155350401,0.5711856968,3.8223783324\N,
0,2.3320498355,0.9995149288,4.1964302526\H,0,1.3460468899,-0.840743708
7,4.1534340912\C,0,2.2174797224,1.0262376234,5.680763416\C,0,2.3195450
836,2.371088517,3.621971243\H,0,1.2393677633,1.4307479307,5.9459516937
\H,0,3.009156648,1.657225818,6.0837569782\H,0,2.3206959489,0.006909946
,6.0538571154\H,0,1.3560853133,2.8324189377,3.847720851\H,0,2.46810237
98,2.3140540722,2.5442983874\H,0,3.1252947656,2.9439150324,4.080390232
7\H,0,-0.2086408508,1.2232682529,1.7209395535\H,0,3.221179268,0.529896
946,3.962374355\\Version=ES64L-G16RevA.03\State=1-A\HF=-941.1774255\RM
SD=4.839e-09\PG=C01 [X(C15H24N1O4)]\@

Meta-

1\1\GINC-R403\SP\RM062X TD-FC\6-31+G(d,p)\C15H24N1O4(1+)\ROOT\21-Jan-2
019\0\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent
=toluene) td(nstates=10,50-50) maxdisk=2684354560\\title\\1,1\C,0,-7.9
854647731,5.421082418,-2.9644667744\C,0,-6.6726929475,5.8071977654,-3.
6009909748\O,0,-5.6709987693,5.1025838104,-2.8634627767\C,0,-4.3857145
022,5.5352602443,-2.9023792276\C,0,-3.6115507162,5.1905102883,-1.78031
36993\C,0,-2.286574494,5.5906755303,-1.73236123\C,0,-4.2483584744,4.41
80471725,-0.6592352281\C,0,-1.7033598341,6.3191312354,-2.7812852876\C,
0,-2.4973320671,6.6518504876,-3.8825544694\H,0,-2.0954565114,7.2230089
392,-4.7092295428\C,0,-3.8376917887,6.2726754013,-3.9464680161\H,0,-4.
4400194473,6.5413854379,-4.8069924988\C,0,-0.2645391575,6.7021305792,-
2.600157565\C,0,0.6165025158,7.2661546629,-3.7323393964\C,0,0.61295334
36,6.3639605256,-4.9676396114\C,0,0.1967010925,8.7083223834,-4.0535179
441\O,0,1.9484150103,7.2964525431,-3.2610287962\O,0,-7.882877491,5.740
8750161,-1.5749207273\O,0,0.2445115527,6.5605648958,-1.4999162787\H,0,
-8.1684989856,4.3480445948,-3.0936994903\H,0,-8.7953995885,5.984492701
6,-3.4388852756\H,0,-6.50102376,6.8860139767,-3.5070793688\H,0,-6.6547
797033,5.5167548714,-4.6568698195\H,0,-0.3379869888,6.3701354062,-5.50
28092471\H,0,0.8559694461,5.3349220151,-4.6875910912\H,0,1.3918082272,
6.7241244288,-5.6452669081\H,0,-0.7903398225,8.7854756492,-4.514068915
\H,0,0.9339526787,9.1212193705,-4.7474750773\H,0,0.2089538433,9.315888
0897,-3.14332579\H,0,1.924587908,7.1788456577,-2.2983551525\H,0,-8.754
0841294,5.6718653667,-1.1650065011\H,0,-4.6325232339,3.4532857671,-1.0
015832883\N,0,-5.4249858513,5.146772023,-0.0588068314\H,0,-3.535061103
3,4.2497900965,0.1514979129\H,0,-1.6763344767,5.3439937859,-0.86801379
66\C,0,-5.0527931227,6.4838529627,0.4804791854\C,0,-6.0831894069,4.313
4819122,0.9831012849\H,0,-6.1258010062,5.2915717633,-0.8081156918\H,0,
-4.3063646977,6.3459241357,1.2650635916\H,0,-5.9486050151,6.9531451919
,0.8878714314\H,0,-4.6447523599,7.0948232318,-0.3235577973\H,0,-5.3715
743572,4.1346120063,1.7907352251\H,0,-6.3935031025,3.3696143487,0.5351
33914\H,0,-6.9516709329,4.8523143098,1.3615205413\\Version=ES64L-G16Re
vA.03\State=1-A\HF=-941.1843437\RMSD=4.188e-09\PG=C01 [X(C15H24N1O4)]\@

Para-

1\1\GINC-R64\SP\RM062X TD-FC\6-31+G(d,p)\C14H22N1O3(1+)\ROOT\18-Apr-20
19\0\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-
50) scrf(smd,solvent=toluene) guess=read geom=allcheck maxdisk=2147483
648\\title\\1,1\C,-1.8856192718,2.4166589201,-1.4464610518\C,-1.033844
6034,1.662202789,-0.4443675632\O,-0.496616504,2.644107456,0.4254866778
\C,0.3554983714,2.2374983413,1.4173706794\C,0.897069557,3.2516999747,2
.2092942326\H,0.6256521869,4.2834013442,2.0105320176\C,1.7680423184,2.
9310736265,3.2396304952\H,2.1726197747,3.7411613418,3.8322748811\C,2.1
229856436,1.5968498746,3.4915017036\C,1.5703910475,0.6001829141,2.6803

403312\H,1.8398307067,-0.4332136477,2.8701173382\C,0.6862127853,0.9024
280507,1.650238862\H,0.2693438893,0.0991033834,1.0543359298\C,3.058731
711,1.1381014277,4.5689216745\C,3.5424872365,2.0471117413,5.7175189612
\C,4.5294066522,3.0962973102,5.1857475432\C,2.371501013,2.675244333,6.
4760672013\O,4.2370536499,1.2345795753,6.642058784\N,-1.1447946724,3.5
976203291,-2.0076815018\O,3.457375301,-0.01547298,4.5538682205\H,-2.78
30208684,2.8160871937,-0.9679533571\H,-2.1712043517,1.7752358226,-2.28
3548184\H,-0.2300628772,1.0977628025,-0.9310262834\H,-1.6758869568,0.9
568981543,0.0961036361\H,4.0649883865,3.8441950496,4.5403426892\H,5.33
96443444,2.6092051976,4.634568632\H,4.9646894013,3.6079455905,6.048602
7397\H,1.820474794,3.4086976136,5.8848618041\H,2.7745235509,3.17463877
28,7.3615608806\H,1.6778181649,1.8982703543,6.810409596\H,4.3837630959
,0.3723405463,6.2213868753\C,-2.0321600659,4.4121605357,-2.8888898267\
C,0.1139314672,3.2185020607,-2.7152390978\H,-2.9231132093,4.6913494508
, -2.3271351021\H,-2.3026820239,3.8081680654,-3.7558327066\H,-1.4897276
862,5.303088878,-3.2036226613\H,0.807345757,2.7684723836,-2.0059738874
\H,0.5550400492,4.1214257814,-3.1360745285\H,-0.1373068739,2.515503004
1,-3.5106186179\H,-0.8797548907,4.1775646374,-1.2019390167\Version=ES
64L-G16RevA.03\State=1-A\HF=-826.6745777\RMSD=5.196e-09\PG=C01 [X(C14H
22N1O3)]\@

I2959- NMe₂H DCM

Ortho-

1\1\GINC-R157\SP\RM062X TD-FC\6-31+G(d,p)\C15H24N1O4(1+)\ROOT\09-Jan-2
019\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent
=dichloromethane) td(nstates=10,50-50) maxdisk=2684354560\title\1,1\
C,0,-6.7410701114,7.4913237347,-1.9067296426\C,0,-5.8123702151,6.70034
80716,-2.8006928799\O,0,-5.9275031637,7.2266382943,-4.1229864321\C,0,-
5.1689463389,6.6910385511,-5.0951194101\C,0,-5.3136448365,7.2635944378
, -6.3685763563\C,0,-4.5777991445,6.8111422976,-7.4528543976\C,0,-4.842
2537734,7.4757647128,-8.7842430858\C,0,-3.6788982866,5.7237773951,-7.2
829220813\C,0,-3.5656681813,5.1532996189,-6.0110041507\H,0,-2.88815702
64,4.3261582689,-5.8420988646\C,0,-4.2807691331,5.6283726691,-4.915986
7576\H,0,-4.1443812867,5.1603969797,-3.9487967296\C,0,-2.8934366743,5.
2163239278,-8.4390047344\C,0,-2.4880639077,3.7335400875,-8.610411024\C
,0,-1.1808960575,3.4735064277,-7.8455568896\C,0,-4.9209565432,3.009072
0889,-8.9339152355\O,0,-2.2425740331,3.5224747428,-9.9909585529\O,0,-6
.3657247444,8.8518793548,-1.7872791456\O,0,-2.5463350277,5.9883467978,
-9.3294828355\H,0,-6.7762521114,6.9982976381,-0.9270364162\H,0,-7.7493
75244,7.48363664,-2.3297521212\H,0,-6.1009768104,5.6418368173,-2.79390
50847\H,0,-4.7732073798,6.7901533613,-2.4575618175\H,0,-1.2854605536,3
.5554592623,-6.7618619218\H,0,-0.4073822366,4.1740735513,-8.1761214957
\H,0,-0.8538385765,2.4578074339,-8.0854496724\H,0,-2.8995988625,7.9193
205145,-9.2839810043\H,0,-5.3569888058,3.9720517049,-8.6427231738\H,0,
-4.7811644167,3.0097842438,-10.0182402248\H,0,-1.8690885383,4.33923076
59,-10.3570818794\H,0,-5.5510621431,8.9068688506,-1.2690189838\H,0,-4.
9013007482,6.7548615544,-9.6011434147\N,0,-3.7693927713,8.4563468791,-
9.1597772871\H,0,-5.7736278811,8.0423307879,-8.7406650997\C,0,-3.59724
4849,2.7510460972,-8.2189861217\C,0,-3.5669138872,9.5690984285,-8.1936
651318\H,0,-3.7386564829,2.7626222051,-7.1349103929\H,0,-5.6484633839,
2.2316028655,-8.684809225\H,0,-3.221858516,1.7546531312,-8.4790789861\
H,0,-3.2066143013,9.1576128943,-7.2522432814\H,0,-4.5190823249,10.0794
617586,-8.0484513379\H,0,-2.8294744806,10.2517272863,-8.6133425057\H,0
, -6.0239682089,8.0766737244,-6.4880947352\H,0,-4.0052970006,8.84900514
49,-10.0772894794\Version=ES64L-G16RevA.03\State=1-A\HF=-941.211596\R
MSD=1.946e-09\PG=C01 [X(C15H24N1O4)]\@

Meta-

1\1\GINC-R158\SP\RM062X TD-FC\6-31+G(d,p)\C15H24N1O4(1+)\ROOT\09-Jan-2
019\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent
=dichloromethane) td(nstates=10,50-50) maxdisk=2684354560\title\1,1\
C,0,4.4225888693,2.0017718209,3.6273972306\C,0,4.5400501414,0.96661143
07,2.5372780241\O,0,3.3240822622,0.2117450922,2.5927380586\C,0,2.90538
89787,-0.4565609746,1.4933154961\C,0,1.5146826422,-0.6560355878,1.4134

496606\C,0,0.9995306159,-1.3393284263,0.3252614441\C,0,0.6299635223,-0.1150600977,2.501713969\C,0,1.8327115353,-1.8285123581,-0.6958530901\C,0,3.2106773342,-1.603355593,-0.5973346503\H,0,3.8963784092,-1.9641387393,-1.3529682421\C,0,3.7522569803,-0.9210296032,0.4900983263\H,0,4.8236114565,-0.7666628486,0.5574370678\C,0,1.1579432171,-2.554314085,-1.8139786383\C,0,1.8747679243,-2.9602199841,-3.118581949\C,0,2.5222067793,-1.7617876753,-3.814653202\C,0,2.8719192924,-4.0930502022,-2.8401904464\O,0,0.8888897221,-3.4563701503,-4.0086493627\O,0,3.2370742379,2.7531491707,3.3602278579\O,0,-0.0246215496,-2.8485508065,-1.7063300843\H,0,5.3085859658,2.6447988581,3.6091481608\H,0,4.3513619713,1.5135573401,4.6061796896\H,0,5.4051183324,0.3178740656,2.7073277358\H,0,4.6224832803,1.4479451033,1.556080283\H,0,3.3922217462,-1.3756656336,-3.2818769742\H,0,1.7932681409,-0.9548409208,-3.9359958147\H,0,2.8439272971,-2.0870830117,-4.8082663359\H,0,3.7103630861,-3.7847166617,-2.2128365377\H,0,3.2658304134,-4.4365091595,-3.8011649023\H,0,2.3604280837,-4.9310639923,-2.3564355875\H,0,0.081706921,-3.6122086456,-3.4909368067\H,0,3.16788589,3.4749733183,4.0009523661\H,0,-0.4206959661,-0.3211660898,2.2846695693\N,0,0.7527624084,1.3774160331,2.662080335\H,0,0.8872324925,-0.541499346,3.4750844573\H,0,-0.0728819834,-1.4942290697,0.2489159\C,0,-0.1188105085,1.851333078,3.7711345507\C,0,0.4648710336,2.1191223869,1.4051077505\H,0,1.7284061486,1.5982146188,2.9310608423\H,0,-1.1580805586,1.6503330771,3.5066620622\H,0,0.0377327758,2.9226454656,3.8972815428\H,0,0.1528968738,1.3181732268,4.6822242841\H,0,-0.5449865695,1.86533342,1.0776242177\H,0,1.1930695031,1.8367126236,0.6452559644\H,0,0.5414818511,3.1856785328,1.6161127777\Version=ES64L-G16RevA.03\State=1-A\HF=-941.2153006\RMSD=8.478e-09\PG=C01 [X(C15H24N1O4)]\@

Para-

1\1\GINC-R66\SP\RM062X TD-FC\6-31+G(d,p)\C14H22N1O3(1+)\ROOT\18-Apr-2019\0\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50) scrf(smd,solvent=dichloromethane) guess=read geom=allcheck maxdisk=2147483648\title\1,1\C,-1.1867110969,2.4819423361,-2.911925628\C,-0.9819707467,2.8838276917,-4.3556776177\O,-0.9100035731,1.6735100108,-5.0991605311\C,-0.6658644874,1.7456021921,-6.4344615881\C,-0.4723224367,2.9426437187,-7.1256214957\H,-0.5195522138,3.9003445422,-6.6209573871\C,-0.2081392909,2.905434375,-8.4944055792\H,-0.0616559988,3.8528805424,-8.9971062265\C,-0.1460570558,1.6932236507,-9.1894148416\C,-0.3579648168,0.5020377795,-8.469884949\H,-0.3137616372,-0.4442978839,-8.9982361925\C,-0.610046244,0.5202489618,-7.1115246295\H,-0.760900209,-0.399040179,-6.5549003701\C,0.1261966867,1.5540996874,-10.6503262399\C,0.5829271855,2.7246641521,-11.547090442\C,-0.5715547859,3.715088021,-11.7490465892\C,1.8499675027,3.395840557,-11.0140261343\O,0.9158875609,2.1841143506,-12.8152783554\N,-2.3410219495,1.5396041027,-2.7462992718\O,-0.0118421614,0.461490422,-11.1839732958\H,-1.3894393855,3.3587265642,-2.2926544593\H,-0.3066496638,1.9588837346,-2.5326593476\H,-0.041883931,3.4425067804,-4.424719907\H,-1.7938105497,3.5149322984,-4.7336190042\H,-0.8621440909,4.2324361201,-10.8329285485\H,-1.4458075252,3.1924008467,-12.1493788335\H,-0.2494594844,4.4611407865,-12.4815555974\H,1.6798844097,3.9640390008,-10.0988743482\H,2.2133132919,4.0831098318,-11.783726518\H,2.6253286197,2.6467660067,-10.8268434784\H,0.5804767262,1.2722147439,-12.8377883106\C,-3.6407532776,2.1194611411,-3.1911124998\C,-2.4285152937,1.0684388376,-1.3333887027\H,-3.6091820326,2.3069980218,-4.2629696898\H,-3.8033211839,3.047032347,-2.6404400874\H,-4.4253335011,1.3984221582,-2.9651974684\H,-1.4784292312,0.6118036455,-1.0580498204\H,-3.2372783811,0.3421503516,-1.2637137554\H,-2.6371609662,1.93253155,-0.7012458833\H,-2.1483597818,0.7210312021,-3.3371273755\Version=ES64L-G16RevA.03\State=1-A\HF=-826.7107448\RMSD=5.432e-09\PG=C01 [X(C14H22N1O3)]\@

I2959- NMe₂H Acetonitrile

Ortho-

1\1\GINC-R1223\SP\RM062X TD-FC\6-31+G(d,p)\C15H24N1O4(1+)\ROOT\09-Jan-2019\0\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=acetonitrile) td(nstates=10,50-50) maxdisk=2684354560\title\1,1\C,

0,-1.7301700033,2.5184591184,-2.2839182471\C,0,-2.1892935897,3.8165320
432,-2.9061241043\O,0,-2.9087470925,4.516838581,-1.8856912781\C,0,-3.4
702591987,5.7041115814,-2.1890042658\C,0,-4.1768104009,6.3307234552,-1
.1525966342\C,0,-4.8037075136,7.5534174286,-1.3443973218\C,0,-5.505199
9148,8.1594343997,-0.151646012\C,0,-4.6999233286,8.2006710148,-2.60339
09154\C,0,-3.9786961403,7.5647639032,-3.6196388389\H,0,-3.8896523399,8
.0248353454,-4.5960328199\C,0,-3.3782912272,6.3231814431,-3.4372151443
\H,0,-2.8422641583,5.8638842719,-4.2588228863\C,0,-5.3537700677,9.5173
727714,-2.8267148259\C,0,-4.7637346566,10.6116068844,-3.7477324902\C,0
, -3.2440303309,10.7047230393,-3.676864395\C,0,-5.2743811038,10.3993697
986,-5.1798137926\O,0,-5.2502612329,11.8584267827,-3.2726121714\O,0,-2
.8248526453,1.7062902319,-1.8932911921\O,0,-6.4024972005,9.7925993969,
-2.2508335144\H,0,-1.0740697247,2.7293271692,-1.4293333542\H,0,-1.1603
145202,1.9540162509,-3.0259346377\H,0,-2.8542489422,3.6216883543,-3.75
58376353\H,0,-1.3300629451,4.4115112054,-3.2373055606\H,0,-2.753583546
2,9.8614632154,-4.1649677952\H,0,-2.9087500638,10.7584454696,-2.636662
5202\H,0,-2.9393683022,11.6218895614,-4.1889994736\H,0,-4.9248802733,9
.4657876834,-5.6260786544\H,0,-4.9153467879,11.2324701646,-5.791174002
7\H,0,-6.3691604842,10.4026803811,-5.1913007945\H,0,-6.1674839921,11.7
267395024,-2.9853389498\H,0,-3.3289984621,2.1882064407,-1.2236241242\H
,0,-5.1874768097,7.6575122219,0.7647696705\N,0,-7.0014980775,8.0193885
457,-0.2025410847\H,0,-5.3000401708,9.2275868078,-0.0621610446\C,0,-7.
617721113,8.6695581278,0.9877926212\C,0,-7.4513340238,6.6075009998,-0.
3374635098\H,0,-7.2878660086,8.1330643333,1.878451698\H,0,-8.700888174
5,8.6127067625,0.8869962701\H,0,-7.2921666754,9.7094111344,1.023284105
9\H,0,-7.054012709,6.0396357052,0.5055481658\H,0,-7.0845615505,6.20140
91052,-1.2789729734\H,0,-8.5407416532,6.5971296607,-0.3249067994\H,0,-
4.2244459231,5.8369785029,-0.1859531191\H,0,-7.3013459214,8.5418102034
, -1.0378776485\\Version=ES64L-G16RevA.03\State=1-A\HF=-941.2151366\RMS
D=7.534e-09\PG=C01 [X(C15H24N1O4)]\@

Meta-

1\1\GINC-R154\SP\RM062X TD-FC\6-31+G(d,p)\C15H24N1O4(1+)\ROOT\09-Jan-2
019\O\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent
=acetonitrile) td(nstates=10,50-50) maxdisk=2684354560\\title\\1,1\C,0
, -1.3604548263,0.3406817897,-2.9624939871\C,0,0.1018213974,0.117666417
2,-2.6452707495\O,0,0.5829005301,-0.7425725323,-3.6853600448\C,0,1.642
5976265,-1.5484728706,-3.4533669212\C,0,1.6861299882,-2.7147426322,-4.
2407455487\C,0,2.7388888898,-3.5971483599,-4.0691948909\C,0,0.58462918
72,-2.9756397035,-5.2301898027\C,0,3.7634475701,-3.3461741051,-3.13898
85265\C,0,3.6916430399,-2.1805744781,-2.3667083087\H,0,4.4486098624,-1
.9450529484,-1.6304227049\C,0,2.6356847904,-1.2841940636,-2.5127201224
\H,0,2.5966180558,-0.3856234767,-1.9069318345\C,0,4.8450649858,-4.3694
235722,-3.0422382734\C,0,6.1186661771,-4.1829170544,-2.1892503971\C,0,
6.8974011784,-2.9335842291,-2.6073033416\C,0,5.7767589319,-4.193552003
7,-0.694106314\O,0,6.9620720481,-5.2965890385,-2.4405838938\O,0,-2.051
888002,-0.90541721,-3.0494962705\O,0,4.7387384412,-5.416284886,-3.6684
858361\H,0,-1.4615116201,0.8161649327,-3.9414935163\H,0,-1.8090386845,
0.9928698281,-2.2069220462\H,0,0.2191964197,-0.3814202801,-1.675969647
8\H,0,0.6552695215,1.0625985589,-2.6418381453\H,0,6.3832039128,-2.0053
133801,-2.3544378283\H,0,7.0873438797,-2.9507716885,-3.6848552054\H,0,
7.8589448115,-2.9481179746,-2.0855690297\H,0,5.2104685752,-3.317852249
8,-0.3729378904\H,0,6.7187690537,-4.2167385014,-0.1382584407\H,0,5.206
1245763,-5.093854381,-0.4454081471\H,0,6.4532112425,-5.9245619934,-2.9
803973475\H,0,-2.2466203206,-1.2218604727,-2.154673536\H,0,0.504778906
7,-2.1679772017,-5.962492225\N,0,-0.7672750822,-3.0766614189,-4.575609
5442\H,0,0.7491139621,-3.9207500418,-5.75240955\H,0,2.7736705245,-4.50
68547455,-4.6615528101\C,0,-0.8181719798,-4.1333153761,-3.5293972334\C
,0,-1.823484323,-3.2898770585,-5.602619387\H,0,-0.9761503517,-2.174771
6737,-4.1114963462\H,0,-0.5467927877,-5.085213842,-3.9894365313\H,0,-1
.8349934374,-4.1748454947,-3.1385363207\H,0,-0.119086495,-3.8831955976
, -2.7315448195\H,0,-1.6368447502,-4.2451384467,-6.0954186232\H,0,-1.77
91898514,-2.4724451784,-6.3221232845\H,0,-2.7914025747,-3.3028933648,-
5.1022367757\\Version=ES64L-G16RevA.03\State=1-A\HF=-941.2211556\RMSD=

9.373e-09\PG=C01 [X(C15H24N1O4)]\@

Para-

1\1\GINC-R70\SP\RM062X TD-FC\6-31+G(d,p)\C14H22N1O3(1+)\ROOT\18-Apr-2019\0\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50) scrf(smd,solvent=acetonitrile) guess=read geom=allcheck maxdisk=21 47483648\title\1,1\C,-1.1784969228,2.4719863714,-2.9036373903\C,-0.9497820834,2.8716739203,-4.3435766217\O,-0.8680638847,1.6602754037,-5.0884394845\C,-0.6324809097,1.7342178907,-6.4220852918\C,-0.4326041282,2.9318289724,-7.1119674844\H,-0.4655277784,3.8881420257,-6.6037506017\C,-0.1814578329,2.8972519227,-8.4828148686\H,-0.0324528558,3.8459094477,-8.982120713\C,-0.1352637355,1.6867246925,-9.1833071902\C,-0.3498428172,0.4945941485,-8.4649358092\H,-0.3177315771,-0.4511801102,-8.9952598577\C,-0.591585167,0.5101205674,-7.1048046347\H,-0.7482428561,-0.4097615348,-6.550486077\C,0.1222732004,1.5527499996,-10.6453892816\C,0.5592327792,2.729536597,-11.5448692717\C,-0.5990203507,3.7196653929,-11.721040938\C,1.8348677344,3.4001292908,-11.0320170135\O,0.8678577913,2.193421253,-12.8226875207\N,-2.3425536869,1.5400787675,-2.7514429149\O,-0.0117115329,0.4600421831,-11.182525274\H,-1.3842003194,3.3530390993,-2.2915582341\H,-0.3080653697,1.9442961651,-2.509205804\H,-0.0075469255,3.4277491347,-4.3985460504\H,-1.7541361336,3.5036001476,-4.7347146937\H,-0.8657430586,4.2388958825,-10.79905203\H,-1.483413282,3.1972158999,-12.099045078\H,-0.2934574311,4.4649511621,-12.4615473089\H,1.6794346995,3.9668551876,-10.113378796\H,2.1841967329,4.0900956228,-11.8059719538\H,2.6136437682,2.6510417338,-10.8588410835\H,0.5476361737,1.2756425673,-12.8308966919\C,-3.6249429541,2.117465721,-3.2449387798\C,-2.4706932558,1.0992218937,-1.3322220697\H,-3.559545813,2.2848221864,-4.318800523\H,-3.7979364035,3.056173582,-2.7167933959\H,-4.4195861051,1.4040329355,-3.0304597888\H,-1.526328501,0.6552709217,-1.0193578496\H,-3.2763808778,0.3687020749,-1.2721660842\H,-2.7030166394,1.9762834481,-0.7268595964\H,-2.1402466907,0.7055224319,-3.3157969493\Version=ES64L-G16RevA.03\State=1-A\HF=-826.7187697\RMSD=2.514e-09\PG=C01 [X(C14H22N1O3)]\@

I2959- NMe₂H Water

Ortho-

1\1\GINC-R444\SP\RM062X TD-FC\6-31+G(d,p)\C15H24N1O4(1+)\ROOT\21-Jan-2019\0\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=h2o) td(nstates=10,50-50) maxdisk=2684354560\title\1,1\C,0,-1.8196130395,2.2719967522,-2.3758612841\C,0,-0.477859853,1.6073848713,-2.1848716251\O,0,-0.4127993045,1.1790782372,-0.8197609112\C,0,0.7047223007,0.5371648258,-0.4044969873\C,0,0.7181321073,0.1363542664,0.9380805822\C,0,1.8181082492,-0.5084039901,1.4840869075\C,0,1.7328833116,-0.9149867133,2.9351532029\C,0,2.9347885166,-0.8034460681,0.6596238433\C,0,2.8918950157,-0.4120301887,-0.6826758714\H,0,3.7320979183,-0.6077063162,-1.3372514487\C,0,1.8040789212,0.2678504311,-1.2208261065\H,0,1.8269690297,0.570115965,-2.2603283864\C,0,4.1223630916,-1.4951589918,1.2266787931\C,0,4.998402769,-2.4707198232,0.4082652126\C,0,4.1953688951,-3.3567596111,-0.5356291631\C,0,6.0978613239,-1.6795897766,-0.3106611021\O,0,5.612296442,-3.3561166187,1.3400116756\O,0,-2.8979989672,1.3560850842,-2.2314603055\O,0,4.4380506502,-1.3182197147,2.4004351454\H,0,-1.8710168079,2.6656706606,-3.3933771616\H,0,-1.9261655802,3.1061392385,-1.6724000926\H,0,0.3288674235,2.3203390413,-2.3899491557\H,0,-0.3798561402,0.7384289366,-2.8454483714\H,0,3.8013976033,-2.8002753567,-1.3863504059\H,0,3.3640502239,-3.8313290554,-0.0060890465\H,0,4.8611583287,-4.136489797,-0.9159708677\H,0,5.7046457607,-0.9738938002,-1.0449395886\H,0,6.7464740641,-2.3930524597,-0.8270305049\H,0,6.6930700991,-1.1256026839,0.4218565105\H,0,5.9040666308,-2.8305446786,2.1017993985\H,0,-2.9300212524,1.0656961583,-1.3095317032\H,0,0.6946817349,-0.9034649219,3.2737959943\N,0,2.4776732619,0.0226211146,3.8446346378\H,0,2.1523501163,-1.9078170887,3.1019627971\C,0,2.5309695454,-0.5366862773,5.2231698752\C,0,1.9081440041,1.3968226307,3.8429709342\H,0,1.5089573848,-0.6425439143,5.5896399083\H,0,3.0918346307,0.1519994429,5.8537524889\H,0,3.0258256092,-1.5069528138,5.1843084667\H,0,0.8676801509,1.3342205232,4.165868

4847\H,0,1.9732912317,1.81258828,2.8386079583\H,0,2.4867562545,2.00527
08738,4.5369099473\H,0,-0.1526709046,0.3452332514,1.5531355116\H,0,3.4
41741249,0.054033075,3.4869708138\Version=ES64L-G16RevA.03\State=1-A\
HF=-941.2099469\RMSD=5.043e-09\PG=C01 [X(C15H24N1O4)]\@

Meta-

1\1\GINC-R732\SP\RM062X TD-FC\6-31+G(d,p)\C15H24N1O4(1+)\ROOT\21-Jan-2
019\0\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent
=h2o) td(nstates=10,50-50) maxdisk=2684354560\title\1,1\C,0,-6.99733
29417,4.0344412033,-7.5190885052\C,0,-6.0525767166,4.7935664421,-6.615
4308927\O,0,-5.0419471752,3.8526841666,-6.2302095425\C,0,-3.8055940123
,4.305858704,-5.9103680529\C,0,-2.7550799346,3.4044083688,-6.159631152
1\C,0,-1.4601642309,3.7894351246,-5.8566781828\C,0,-3.0573307038,2.063
8058,-6.7668907699\C,0,-1.1806004323,5.0577196764,-5.3188680775\C,0,-2
.2440635068,5.9400374179,-5.0921388532\H,0,-2.080956418,6.9218045532,-
4.6658103603\C,0,-3.554815756,5.569814933,-5.3804270175\H,0,-4.3710528
263,6.2561724071,-5.1842984182\C,0,0.2484193786,5.361292028,-5.0328114
336\C,0,0.7879474518,6.7949740558,-4.8557252942\C,0,0.3170677522,7.747
1617631,-5.9509561699\C,0,0.4454990479,7.2937262553,-3.4465142971\O,0,
2.205216062,6.7303158947,-4.9787369141\O,0,-6.303312078,3.4858358271,-
8.6385612758\O,0,1.0531459779,4.4403471835,-4.9344397408\H,0,-7.804505
8198,4.699227229,-7.8425494034\H,0,-7.4309495512,3.1863345056,-6.98392
15052\H,0,-6.5742165797,5.1769821408,-5.7327830248\H,0,-5.5850733026,5
.6238657552,-7.1571406788\H,0,-0.7399567831,7.9979575496,-5.8621415018
\H,0,0.4972512338,7.3136192365,-6.9389925612\H,0,0.8949526614,8.671758
6708,-5.8638737808\H,0,-0.6287511107,7.3864951543,-3.2768200255\H,0,0.
903753576,8.2781132558,-3.3143739342\H,0,0.8602411448,6.6085718519,-2.
7008031804\H,0,2.4882924553,5.8625921283,-4.6466472489\H,0,-5.99912641
65,4.2114551061,-9.2037129688\H,0,-2.1371965642,1.4960529904,-6.921372
9016\N,0,-3.7256452488,2.1730732784,-8.1100616872\H,0,-3.73761992,1.48
29579553,-6.1389159123\H,0,-0.641670084,3.1051783898,-6.0603889384\C,0
,-3.9719394872,0.8177461011,-8.6715195129\C,0,-2.9590995319,3.01557101
07,-9.0671170681\H,0,-4.647779139,2.6282035819,-7.9864885654\H,0,-3.00
83303826,0.3455995887,-8.8678748818\H,0,-4.5375780823,0.9263889385,-9.
5964790165\H,0,-4.5404847216,0.237362525,-7.9451882898\H,0,-1.94939848
84,2.6095095123,-9.152597863\H,0,-2.9278341476,4.0407699199,-8.6983097
024\H,0,-3.467210648,2.9813018193,-10.0309058965\Version=ES64L-G16Rev
A.03\State=1-A\HF=-941.2154082\RMSD=7.431e-09\PG=C01 [X(C15H24N1O4)]\@

Para-

1\1\GINC-R69\SP\RM062X TD-FC\6-31+G(d,p)\C14H22N1O3(1+)\ROOT\18-Apr-20
19\0\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-
50) scrf(smd,solvent=h2o) guess=read geom=allcheck maxdisk=2147483648\
\title\1,1\C,-1.1726360986,2.4633635175,-2.8989187197\C,-0.9261184493
,2.8566424756,-4.3360275005\O,-0.8116813905,1.6420168746,-5.0742344161
\C,-0.5920007405,1.7204764233,-6.4132317706\C,-0.4257075261,2.92218312
93,-7.104720232\H,-0.4706475202,3.8773185029,-6.5959492371\C,-0.194443
506,2.8927605406,-8.4783117789\H,-0.0765392754,3.8447134649,-8.9796204
421\C,-0.1372204757,1.6825854957,-9.1796841548\C,-0.3144573689,0.48574
88573,-8.4588348098\H,-0.2693385348,-0.4611884544,-8.9856586631\C,-0.5
332356585,0.4970920266,-7.0950570898\H,-0.6601305933,-0.4250528644,-6.
5373983455\C,0.0854396437,1.5599108768,-10.6448276368\C,0.5579489454,2
.7299324079,-11.5317736501\C,-0.5977065513,3.717004855,-11.7382467277\
C,1.8218064843,3.4000695705,-10.997377358\O,0.9082372992,2.1845709123,
-12.7998222869\N,-2.3437347426,1.5395961928,-2.7577960231\O,-0.1160365
073,0.483151249,-11.2005294213\H,-1.3802043573,3.3484594011,-2.2934537
309\H,-0.3088767218,1.9342177334,-2.492373524\H,0.0077678913,3.4263465
29,-4.3824392279\H,-1.7358819165,3.4695383399,-4.7444583415\H,-0.91390
29257,4.2037943512,-10.8143339847\H,-1.456742263,3.1960333557,-12.1718
550485\H,-0.2634233517,4.4870285534,-12.4396058738\H,1.64041912,3.9845
751685,-10.0956662644\H,2.1958601397,4.0758704058,-11.771955626\H,2.59
04357052,2.6509588711,-10.7861304911\H,0.4247120372,1.3473126449,-12.8
983951337\C,-3.6133051843,2.1274870784,-3.2714188262\C,-2.4946643664,1
.1112850876,-1.3376079078\H,-3.5353259899,2.274771082,-4.3471527333\H,

-3.7775510212,3.0772513059,-2.7606057629\H,-4.421109263,1.4305600247,-
3.0522799457\H,-1.5560783328,0.670356266,-1.0042683151\H,-3.3011622725
,0.3815406574,-1.2821437105\H,-2.736230039,1.9938465614,-0.7441096065\
H,-2.1394493221,0.7041555286,-3.3190366816\\Version=ES64L-G16RevA.03\S
tate=1-A\HF=-826.7104339\RMSD=5.097e-09\PG=C01 [X(C14H22N1O3)]\@

I2959-MgCl₂ Gas

1\1\GINC-R136\SP\RM062X TD-FC\6-31+G(d,p)\C12H16Cl2Mg1O4\ROOT\30-Jan-2
019\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50
-50) guess=read geom=allcheck maxdisk=2147483648\\title\0,1\C,0,-3.47
60237406,2.4083166592,6.3151208619\C,0,-2.1519307618,1.7139798088,6.55
72543207\O,0,-1.8148925753,1.0679754261,5.3295294532\C,0,-0.6456276424
,0.4057915322,5.2372800362\C,0,0.2757626912,0.2883173305,6.2856607057\
H,0,0.0880210157,0.7407202684,7.2511664001\C,0,1.4472941258,-0.4253254
068,6.0810076732\H,0,2.1642288044,-0.5295967864,6.8881754764\C,0,1.738
673504,-1.0184944164,4.8440208432\C,0,0.7988292679,-0.8907854845,3.803
876549\H,0,0.9624446542,-1.3542503879,2.8390678249\C,0,-0.3783070604,-
0.1950417122,3.9976140902\H,0,-1.1153012097,-0.1038146696,3.2076264769
\C,0,3.010860684,-1.7559098245,4.7428933398\C,0,3.6127235044,-2.241428
1351,3.403338258\C,0,2.8557724477,-3.4791683293,2.9166922489\C,0,3.72
27388447,-1.1278807318,2.3634979729\O,0,4.9377141999,-2.7111448105,3.6
901769254\O,0,-3.3637240346,3.4011281712,5.3222171554\O,0,3.6396497818
, -2.0097827869,5.7725450964\H,0,-3.7907767772,2.9106303746,7.233178183
5\H,0,-4.2363125679,1.6603788984,6.0519987244\H,0,-2.2358394567,0.9708
774949,7.3602496862\H,0,-1.3792236057,2.4507656857,6.8074142747\H,0,1.
8042455175,-3.2670293127,2.7193671835\H,0,2.9227904429,-4.2707276317,3
.6699079656\H,0,3.3294582581,-3.8324342504,1.9975897524\H,0,2.75100660
33,-0.7859841983,2.0106236611\H,0,4.283593282,-1.5136393412,1.50798815
93\H,0,4.253314976,-0.2624115259,2.7752110094\H,0,5.595729425,-1.99477
01166,3.6400998194\H,0,-3.089196654,2.9758238312,4.5007758853\Mg,0,5.2
571218497,-3.2761437239,5.684113911\C1,0,4.4163707349,-5.3157373153,6.
0511911167\C1,0,7.1153514713,-1.9981645831,5.8128533913\\Version=ES64L
-G16RevA.03\State=1-A\HF=-1888.111068\RMSD=9.971e-10\PG=C01 [X(C12H16C
l2Mg1O4)]\@

I2959- MgCl₂ Toluene

1\1\GINC-R116\SP\RM062X TD-FC\6-31+G(d,p)\C12H16Cl2Mg1O4\ROOT\30-Jan-2
019\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent
=toluene) td(nstates=10,50-50) guess=read geom=allcheck maxdisk=214748
3648\\title\0,1\C,0,-3.4724394283,2.4198158344,6.315214944\C,0,-2.154
6633204,1.7174974704,6.5551364813\O,0,-1.81458566,1.076517815,5.322474
7881\C,0,-0.6524504247,0.4064203482,5.232839288\C,0,0.2600161115,0.273
6120831,6.2883905263\H,0,0.0691224269,0.7227894057,7.2550989197\C,0,1.
4253168369,-0.4496491816,6.087696627\H,0,2.1324438619,-0.5594543469,6.
9028137376\C,0,1.7216520091,-1.0379761086,4.8474303592\C,0,0.791409714
1,-0.891202296,3.7992120767\H,0,0.9557536256,-1.3447024888,2.829879336
7\C,0,-0.3801220105,-0.1863940025,3.989608099\H,0,-1.1075138427,-0.082
5117175,3.1918066538\C,0,2.9866561804,-1.7786439183,4.7452936368\C,0,3
.5885150871,-2.2593920745,3.4047279581\C,0,2.8145663903,-3.4700674488,
2.882423822\C,0,3.7369184877,-1.1313264272,2.3871106151\O,0,4.90871133
82,-2.7557639097,3.7066713203\O,0,-3.3569757666,3.4251473411,5.3299261
027\O,0,3.6162290333,-2.0404702975,5.7778233496\H,0,-3.7848292481,2.91
27697036,7.2393676777\H,0,-4.2381864444,1.6812018621,6.04240708\H,0,-2
.2500367785,0.9705105995,7.352573782\H,0,-1.377077576,2.4449969911,6.8
157458147\H,0,1.7800043396,-3.2259492274,2.6392214474\H,0,2.8181319149
, -4.2703754996,3.6285683376\H,0,3.3146063351,-3.8340616555,1.981272696
1\H,0,2.7761896285,-0.7589541327,2.0339961274\H,0,4.2890839561,-1.5144
163963,1.5237627523\H,0,4.2869110805,-0.2874284745,2.8183043729\H,0,5.
5838627043,-2.0887825414,3.4946353146\H,0,-3.0864925144,3.0048883571,4
.5035186568\Mg,0,5.2821514974,-3.2103231805,5.7001503811\C1,0,4.690013
2679,-5.3262233477,6.2189104443\C1,0,7.1536471874,-1.9170591381,5.8273
064731\\Version=ES64L-G16RevA.03\State=1-A\HF=-1888.1439469\RMSD=1.407
e-09\PG=C01 [X(C12H16Cl2Mg1O4)]\@

I2959- MgCl₂ DCM

```
1\1\GINC-R127\SP\RM062X TD-FC\6-31+G(d,p)\C12H16Cl2Mg1O4\ROOT\30-Jan-2
019\0\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent
=dichloromethane) td(nstates=10,50-50) guess=read geom=allcheck maxdis
k=2147483648\title\0,1\C,0,-3.5117914563,2.3597320197,6.3381944528\C
,0,-2.197928058,1.6514234751,6.5762100578\O,0,-1.8154215553,1.08631209
5,5.3168233981\C,0,-0.6480339182,0.4290104592,5.2214991443\C,0,0.22258
52095,0.2160879093,6.3004345556\H,0,-0.0109157928,0.5857805216,7.29123
60536\C,0,1.3995954285,-0.4833872294,6.0888477559\H,0,2.0732403914,-0.
6512185699,6.9220805101\C,0,1.745382112,-0.9821948869,4.8203014625\C,0
,0.8558502716,-0.7554279318,3.7493818298\H,0,1.0614082955,-1.117421825
,2.7506922469\C,0,-0.321934996,-0.0628346444,3.9468059875\H,0,-1.01014
68985,0.1114059983,3.1265699517\C,0,3.0132937256,-1.7119681449,4.71802
91036\C,0,3.5598388476,-2.2738780887,3.3970163072\C,0,2.667112802,-3.3
890671539,2.8532018973\C,0,3.8612135343,-1.1636077772,2.390847177\O,0,
4.8220051102,-2.8706762823,3.7708528989\O,0,-3.3756141062,3.4293204017
,5.4195604305\O,0,3.6898306014,-1.8936547277,5.742011346\H,0,-3.855916
6231,2.7903070898,7.2818325404\H,0,-4.2628854022,1.6374523063,5.992405
5986\H,0,-2.3170642079,0.8578483403,7.3231668758\H,0,-1.4309964137,2.3
620006869,6.9053597707\H,0,1.7013841113,-3.0166492772,2.5128850126\H,0
,2.5044964497,-4.1510897166,3.6207000466\H,0,3.171610719,-3.8504724802
,1.9985885604\H,0,2.9565165111,-0.6777054241,2.0257785952\H,0,4.377912
7204,-1.6061598419,1.5331685329\H,0,4.5106616942,-0.4098597272,2.84442
40821\H,0,5.2478527647,-3.2609049041,2.9907055529\H,0,-3.1081113814,3.
0618453561,4.5656606043\Mg,0,5.4098955925,-2.9487856891,5.716293235\Cl
,0,5.0777805631,-5.0388857624,6.5833194121\Cl,0,7.2438333541,-1.627636
5746,6.0364350135\Version=ES64L-G16RevA.03\State=1-A\HF=-1888.1636365
\RMSD=4.154e-09\PG=C01 [X(C12H16Cl2Mg1O4)]\@
```

I2959- MgCl₂ Acetonitrile

```
1\1\GINC-R125\SP\RM062X TD-FC\6-31+G(d,p)\C12H16Cl2Mg1O4\ROOT\30-Jan-2
019\0\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent
=acetonitrile) td(nstates=10,50-50) guess=read geom=allcheck maxdisk=2
147483648\title\0,1\C,0,-3.5191294911,2.3367484016,6.3471310938\C,0,
-2.1880188639,1.6591610065,6.5758247502\O,0,-1.8115928871,1.0846491021
,5.318065456\C,0,-0.637956448,0.4395844253,5.2196443159\C,0,0.24866293
78,0.2578659419,6.2919070756\H,0,0.0240700229,0.6459117192,7.277821090
5\C,0,1.4290225053,-0.4356937088,6.0796656574\H,0,2.113490863,-0.58043
8033,6.9084259042\C,0,1.7637099466,-0.9558705741,4.8164431776\C,0,0.86
03646534,-0.7567345061,3.7515645966\H,0,1.0584697348,-1.1362013038,2.7
580455305\C,0,-0.3220711972,-0.0724407087,3.9502262346\H,0,-1.02172813
05,0.077780746,3.1348489171\C,0,3.0304485989,-1.6846340752,4.710776445
2\C,0,3.5718701361,-2.2460756582,3.3877952428\C,0,2.6998867235,-3.3920
232987,2.8748603318\C,0,3.8275353944,-1.148469319,2.3565339538\O,0,4.8
583230727,-2.8029388257,3.75056489\O,0,-3.4200219367,3.3891818761,5.40
24333415\O,0,3.7093667911,-1.8711693827,5.7339926856\H,0,-3.8540932091
,2.7803454692,7.2878958325\H,0,-4.262356342,1.5937794543,6.0297744736\
H,0,-2.280051084,0.8738902963,7.3349219189\H,0,-1.4302175965,2.3882246
662,6.8845649171\H,0,1.7170182361,-3.0473008469,2.5544923571\H,0,2.575
0633012,-4.1505373995,3.6530609958\H,0,3.1975897242,-3.8453244298,2.01
16798065\H,0,2.9018692026,-0.7149670258,1.9783890678\H,0,4.3626709806,
-1.5901312925,1.50981475\H,0,4.4418994775,-0.3551546638,2.7907036904\H
,0,5.2673207028,-3.2139291599,2.970901874\H,0,-3.1584718678,3.00614877
,4.5540856211\Mg,0,5.3846138095,-2.9964836868,5.698610077\Cl,0,4.90088
5893,-5.0825124906,6.5246110299\Cl,0,7.268096346,-1.8192014851,6.24124
28978\Version=ES64L-G16RevA.03\State=1-A\HF=-1888.1667553\RMSD=2.042e
-09\PG=C01 [X(C12H16Cl2Mg1O4)]\@
```

I2959- MgCl₂ Water

```
1\1\GINC-R139\SP\RM062X TD-FC\6-31+G(d,p)\C12H16Cl2Mg1O4\ROOT\30-Jan-2
019\0\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent
=h2o) td(nstates=10,50-50) guess=read geom=allcheck maxdisk=2147483648
\title\0,1\C,0,-3.5323893187,2.3316806696,6.3429360843\C,0,-2.235886
8192,1.5902170928,6.5624534054\O,0,-1.8016620992,1.1263085262,5.277740
3699\C,0,-0.6354293869,0.4535723886,5.1921694931\C,0,0.1774942637,0.15
59747625,6.2948291683\H,0,-0.0998349462,0.4613584167,7.2959239741\C,0,
```

1.3548795478,-0.5463203017,6.092205665\H,0,1.9833410907,-0.7787200111,
6.9447888259\C,0,1.7501542518,-0.971705335,4.811961219\C,0,0.917251306
4,-0.6603104446,3.7182379585\H,0,1.1727702659,-0.9509591063,2.70829540
04\C,0,-0.2561664137,0.0438508929,3.9047046727\H,0,-0.8979858895,0.288
4456287,3.0651548235\C,0,3.0131432862,-1.7123780033,4.7132842754\C,0,3
.5182480966,-2.3443780803,3.4091586701\C,0,2.5387453321,-3.3684820841,
2.8387710733\C,0,3.9336353416,-1.2661855243,2.4081321352\O,0,4.7042392
781,-3.0607172253,3.8059531774\O,0,-3.3506358604,3.5089451221,5.566360
1172\O,0,3.7188825943,-1.8398151085,5.7275857681\H,0,-3.9212811966,2.6
474476576,7.3134992174\H,0,-4.2663767131,1.6679283506,5.8711202613\H,0
, -2.3949209034,0.7372859884,7.2315406189\H,0,-1.4764047437,2.257421613
8,6.9847545153\H,0,1.6482066511,-2.9026050764,2.4182162313\H,0,2.23977
07108,-4.0807535935,3.6122951152\H,0,3.0513054985,-3.9092572339,2.0376
139153\H,0,3.0801917141,-0.7014638683,2.033498177\H,0,4.4176372758,-1.
7603738201,1.5600388276\H,0,4.6439840401,-0.5758925038,2.8715641067\H,
0,5.1644148834,-3.4050504663,3.0257408247\H,0,-3.0954031315,3.24658606
19,4.6712218906\Mg,0,5.4791027244,-2.8482029197,5.6547556885\C1,0,5.48
44379894,-4.7849951868,6.8953527116\C1,0,7.2790812789,-1.4134172789,5.
8094616218\\Version=ES64L-G16RevA.03\State=1-A\HF=-1888.1637666\RMSD=2
.196e-09\PG=C01 [X(C12H16Cl2Mg1O4)]\@

I2959-CaCl₂ Gas

1\1\GINC-R232\SP\RM062X TD-FC\6-31+G(d,p)\C12H16Ca1Cl2O4\ROOT\30-Jan-2
019\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50
-50) guess=read geom=allcheck maxdisk=2147483648\title\0,1\C,0,-3.51
69722009,2.3869133171,6.3083389242\C,0,-2.2333729122,1.6232289778,6.55
96118957\O,0,-1.817514638,1.1220891521,5.2891469852\C,0,-0.6610780245,
0.4370856343,5.201759117\C,0,0.1728168848,0.1590056849,6.2919925206\H,
0,-0.0784973878,0.4936136331,7.2905496518\C,0,1.3400206987,-0.56120689
47,6.0854183244\H,0,1.9892108154,-0.784506414,6.9246602617\C,0,1.71124
21464,-1.0170106808,4.8116556536\C,0,0.8569054557,-0.7268277967,3.7304
083956\H,0,1.0857917445,-1.0593616862,2.7264418521\C,0,-0.3104623973,-
0.0135477874,3.9203368329\H,0,-0.9750850515,0.2080918584,3.092840065\C
,0,2.9754637121,-1.7794180807,4.7197139491\C,0,3.5489531967,-2.3111721
631,3.3842586471\C,0,2.6328682803,-3.3931408954,2.8066604214\C,0,3.851
6232768,-1.1680136121,2.4113152532\O,0,4.7795484862,-2.9751791942,3.67
24142077\O,0,-3.302977431,3.4902976481,5.459390006\O,0,3.6007738367,-2
.019732261,5.7537176363\H,0,-3.8905446716,2.7824837157,7.2560609551\H,
0,-4.2723070683,1.7034850207,5.8970953277\H,0,-2.3981632889,0.79019519
96,7.2546230926\H,0,-1.4645924759,2.2966068454,6.9571060084\H,0,1.6384
6774,-3.0219023546,2.5601390984\H,0,2.5274935813,-4.2108268852,3.52551
09202\H,0,3.1018808228,-3.7889268035,1.9028683428\H,0,2.9609408295,-0.
6223361208,2.1034533164\H,0,4.3240014497,-1.59171004,1.5205690235\H,0,
4.5464237152,-0.4563938108,2.8707451624\H,0,5.5363449001,-2.368752313,
3.5191849863\H,0,-2.9707598365,3.1611582182,4.6153932096\Ca,0,5.592443
936,-3.2817786323,5.9574453158\C1,0,5.1940275198,-5.2913969655,7.50101
27798\C1,0,7.2316243554,-1.5760735133,4.7894818597\\Version=ES64L-G16R
evA.03\State=1-A\HF=-2365.6060086\RMSD=4.076e-09\PG=C01 [X(C12H16Ca1Cl
2O4)]\@

I2959- CaCl₂ Toluene

1\1\GINC-R257\SP\RM062X TD-FC\6-31+G(d,p)\C12H16Ca1Cl2O4\ROOT\30-Jan-2
019\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent
=toluene) td(nstates=10,50-50) guess=read geom=allcheck maxdisk=214748
3648\title\0,1\C,0,-6.936777752,-0.7991166878,0.4023168105\C,0,-5.46
65739943,-0.9563900674,0.7208973532\O,0,-4.7710764155,-0.0883472729,-0
.1763261561\C,0,-3.428169734,-0.0102349676,-0.1000415349\C,0,-2.651477
3098,-0.7314948482,0.8153230749\H,0,-3.1065798006,-1.4042396885,1.5315
182225\C,0,-1.2726303581,-0.5842829045,0.7955111157\H,0,-0.6665395237,
-1.1475650525,1.4961512264\C,0,-0.6316826949,0.2680583253,-0.116307563
3\C,0,-1.4330220457,0.9857616413,-1.0251871538\H,0,-0.999943062,1.6564
233323,-1.7559177465\C,0,-2.8084625204,0.8515272199,-1.0169180196\H,0,
-3.4277902858,1.3992882285,-1.7189880901\C,0,0.8461630359,0.3170331111
, -0.0546848142\C,0,1.7130791313,1.1448841342,-1.0340367109\C,0,1.54826
48248,0.6353968879,-2.4654456186\C,0,1.4556150956,2.6442449334,-0.8764

031131\O,0,3.0850189889,0.8974794314,-0.705302493\O,0,-7.3840402453,0.5198605734,0.6376375423\O,0,1.4283916993,-0.3466804489,0.8044539323\H,0,-7.5153300174,-1.4550718571,1.0579896004\H,0,-7.1209577026,-1.1016511824,-0.6375404665\H,0,-5.1443170575,-1.9936068252,0.5664325847\H,0,-5.2661119367,-0.6532420761,1.7555674761\H,0,0.5309583477,0.7554117631,-2.8376815789\H,0,1.8124559555,-0.4255689746,-2.5176163051\H,0,2.2302311031,1.1965471159,-3.1095388506\H,0,0.4491658746,2.9357036978,-1.1745529476\H,0,2.1690571692,3.1845513141,-1.5056620283\H,0,1.6008387624,2.9512747892,0.1656719766\H,0,3.4214744924,1.5666091955,-0.0806884662\H,0,-6.8706263445,1.1133105629,0.0744046566\Ca,0,3.721403417,-1.0250330102,0.6577069783\Cl,0,3.1027999524,-3.0494144402,-0.9207757682\Cl,0,4.8495109502,1.0639940468,1.8846928748\Version=ES64L-G16RevA.03\State=1-A\HF=-2365.6559579\RMSD=4.787e-09\PG=C01 [X(C12H16CaCl2O4)]\@

I2959- CaCl₂ DCM

1\1\GINC-R152\SP\RM062X TD-FC\6-31+G(d,p)\C12H16CaCl2O4\ROOT\30-Jan-2019\O\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=dichloromethane) td(nstates=10,50-50) guess=read geom=allcheck maxdisk=2147483648\title\0,1\C,0,-4.4509932463,0.1775879411,6.4753481905\C,0,-3.1208272959,-0.5173320761,6.6559175044\O,0,-2.419868011,-0.3578605405,5.4192618423\C,0,-1.162574255,-0.8307983047,5.3141050892\C,0,-0.4988937864,-1.5309555127,6.3304469149\H,0,-0.9812428327,-1.7333579622,7.279209551\C,0,0.7972871678,-1.9758343806,6.1088746982\H,0,1.3131336366,-2.521720729,6.8918756729\C,0,1.4595645701,-1.7489058048,4.8922419998\C,0,0.7718015646,-1.0449850935,3.8845192185\H,0,1.2281190602,-0.8308446599,2.9269505407\C,0,-0.5172013771,-0.5903024487,4.0921767458\H,0,-1.0462697354,-0.0438846014,3.3183673156\C,0,2.8413861065,-2.2690323601,4.7730630942\C,0,3.6275628908,-2.2511075493,3.4469328864\C,0,2.8927728407,-3.0127982775,2.3416980394\C,0,4.0068469423,-0.8199467756,3.0572302351\O,0,4.8302397614,-2.9687311258,3.7327803371\O,0,-4.2901968648,1.5654465726,6.2405927957\O,0,3.3910908879,-2.748015272,5.7650978894\H,0,-5.033606488,0.073489578,7.3940380257\H,0,-5.0066453987,-0.297405302,5.6560654089\H,0,-3.2667633377,-1.5820621372,6.8730346158\H,0,-2.5477519729,-0.0480025366,7.4641598909\H,0,1.9711495767,-2.5232042689,2.0268438111\H,0,2.6540170633,-4.0248597297,2.68155518\H,0,3.5594842154,-3.0838535208,1.477330751\H,0,3.1408248811,-0.2032933149,2.8185445372\H,0,4.6451362213,-0.8592989866,2.1679451064\H,0,4.5634529592,-0.3420933848,3.8695918466\H,0,5.5878551599,-2.5988784454,3.2491123562\H,0,-3.7823014977,1.6742198875,5.4243272499\Ca,0,5.6159247168,-3.7940291983,5.8952163781\Cl,0,4.4575096232,-5.8462121974,7.2976973085\Cl,0,7.7992162535,-2.7524374821,4.4651969725\Version=ES64L-G16RevA.03\State=1-A\HF=-2365.6934865\RMSD=1.659e-09\PG=C01 [X(C12H16CaCl2O4)]\@

I2959- CaCl₂ Acetonitrile

1\1\GINC-R78\SP\RM062X TD-FC\6-31+G(d,p)\C12H16CaCl2O4\ROOT\30-Jan-2019\O\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent=acetonitrile) td(nstates=10,50-50) guess=read geom=allcheck maxdisk=2147483648\title\0,1\C,0,-3.6214631612,2.4148527449,6.2285191027\C,0,-2.326830388,1.6888966942,6.5131687948\O,0,-1.9344168418,1.0759912052,5.2808374659\C,0,-0.7638556295,0.4112301168,5.2248708996\C,0,0.0841858458,0.2200686513,6.3243437417\H,0,-0.1687617957,0.6097871933,7.303150171\C,0,1.2683835894,-0.4834001865,6.1493490517\H,0,1.9266916867,-0.6322398657,6.9988600388\C,0,1.6446225039,-0.9985885702,4.8992579356\C,0,0.7758370766,-0.796942355,3.8097197103\H,0,1.0039246559,-1.1804178691,2.8241445204\C,0,-0.4128039253,-0.1087343437,3.9701517981\H,0,-1.0856264367,0.0418058839,3.132190014\C,0,2.9388382329,-1.7148384899,4.8260414365\C,0,3.5832002949,-2.1249174326,3.4893727642\C,0,2.8066587715,-3.2697579451,2.8305812003\C,0,3.7947349768,-0.9243033015,2.5658964311\O,0,4.8662956067,-2.6263310984,3.8722013816\O,0,-3.44961364,3.4430737941,5.2673591464\O,0,3.5392876435,-1.9858677137,5.8660342065\H,0,-3.9690316767,2.890835454,7.1486627568\H,0,-4.3834733167,1.6958281589,5.9002661806\H,0,-2.4752856391,0.9249753178,7.2852917919\H,0,-1.5513753085,2.3941496049,6.8343899704\H,0,1.8205239716,-2.9670478276,2.4775332627\H,0,2.6904464685,-4.0980932732,3.5359097913\H,0,3.3838880672,-3.6209026275,1.9694538795\H,0,2.8560128106,-0.5059137716,2.2035512592\H,0,4.37407501

92,-1.2532746931,1.6964525455\H,0,4.3531600778,-0.140668528,3.08632532
21\H,0,5.4636955557,-2.6785284756,3.109088983\H,0,-3.1528285235,3.0335
730939,4.4431182533\Ca,0,5.7324456888,-3.2197510702,6.0571152333\C1,0,
5.8021156293,-5.7770685029,7.292712928\C1,0,7.8928821095,-3.1024399725
,4.2553980316\\Version=ES64L-G16RevA.03\State=1-A\HF=-2365.701895\RMSD
=1.160e-09\PG=C01 [X(C12H16Ca1Cl2O4)]\@

I2959- Ca Water

1\1\GINC-R87\SP\RM062X TD-FC\6-31+G(d,p)\C12H16Ca1O4(2+)\ROOT\31-Jan-2
019\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent
=h2o) td(nstates=10,50-50) guess=read geom=allcheck maxdisk=2147483648
\title\2,1\C,0,-3.4199487259,2.4860407834,6.3308879703\C,0,-2.121735
7848,1.7446376419,6.5396537176\O,0,-1.8214746879,1.0805841986,5.307069
1937\C,0,-0.6681918991,0.3762121398,5.2156683806\C,0,0.2522880201,0.24
56735641,6.2625554864\H,0,0.08354538,0.7170299931,7.2229850164\C,0,1.4
029643623,-0.5044371541,6.0580774937\H,0,2.118550193,-0.603969487,6.86
73987886\C,0,1.6731415438,-1.1200167112,4.8274850853\C,0,0.7335605955,
-0.9780504836,3.7899590881\H,0,0.8766395591,-1.4553011769,2.8285000052
\C,0,-0.4250426891,-0.2463923896,3.9831935739\H,0,-1.1578893798,-0.144
7625435,3.1896471011\C,0,2.9320222196,-1.8962753588,4.7244036473\C,0,3
.587375814,-2.2613832069,3.3734864148\C,0,2.8800824518,-3.4779808839,2
.7800439879\C,0,3.6614092295,-1.078397517,2.4115547168\O,0,4.922221818
7,-2.6978341678,3.65237994\O,0,-3.2880200495,3.5310105322,5.3747061671
\O,0,3.4952112292,-2.2676019053,5.7542859453\H,0,-3.7115051389,2.95338
13213,7.273997711\H,0,-4.2066644826,1.7845394471,6.0292349739\H,0,-2.2
280195323,1.0081418619,7.3441964307\H,0,-1.3163771958,2.4463487785,6.7
845275391\H,0,1.8317084387,-3.2737402944,2.5586433616\H,0,2.9322988887
, -4.3172065842,3.4803685234\H,0,3.3870071392,-3.7553483193,1.851800788
\H,0,2.6813280766,-0.7676550952,2.05161472\H,0,4.2638903831,-1.3794539
532,1.5501192718\H,0,4.140455929,-0.2214934584,2.8969255079\H,0,5.4895
596392,-1.9181327197,3.7611410255\H,0,-3.0905491334,3.1329250641,4.515
5073225\Ca,0,5.3607677878,-3.9837419159,5.7594411045\\Version=ES64L-G1
6RevA.03\State=1-A\HF=-1445.01193\RMSD=2.178e-09\PG=C01 [X(C12H16Ca1O4
)]\@

I2959-ZnCl₂ Gas

1\1\GINC-R111\SP\RM062X TD-FC\6-31+G(d,p)\C12H16Cl2O4Zn1\ROOT\30-Jan-2
019\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50
-50) guess=read geom=allcheck maxdisk=2147483648\\title\0,1\C,0,-3.47
5050867,2.4094153761,6.3169689027\C,0,-2.1449997629,1.7245630806,6.553
383139\O,0,-1.8185183332,1.0647623877,5.3308164112\C,0,-0.6468550968,0
.4047098216,5.2360197369\C,0,0.2857473303,0.3061591662,6.2758140874\H,
0,0.1069444456,0.7724560168,7.2364439836\C,0,1.4576917402,-0.407430600
3,6.0697593908\H,0,2.1827816091,-0.4981110301,6.8713483501\C,0,1.73895
10467,-1.0177909394,4.8394784656\C,0,0.7881179111,-0.9086015298,3.8080
170189\H,0,0.9431082697,-1.3858416261,2.8484682406\C,0,-0.3900766634,-
0.2137981749,4.0034847544\H,0,-1.1353137759,-0.1375555682,3.2196107319
\C,0,3.0151755002,-1.757100986,4.7395556443\C,0,3.617064559,-2.2315143
249,3.3952879878\C,0,2.8701384231,-3.474613282,2.9070705108\C,0,3.7007
390971,-1.1101641595,2.3601806523\O,0,4.9479375365,-2.6889185195,3.658
2840146\O,0,-3.3788471598,3.3884238037,5.3085955677\O,0,3.6366473812,-
2.0085162336,5.7711428626\H,0,-3.7819640371,2.9234121049,7.2312124646\
H,0,-4.2346592703,1.654347154,6.0728485651\H,0,-2.2165783005,0.9917817
897,7.3670916807\H,0,-1.3733129295,2.4682199811,6.7860996753\H,0,1.814
0459147,-3.2749971892,2.7217515363\H,0,2.9539910667,-4.2699080278,3.65
42322347\H,0,3.3386796976,-3.8160286248,1.9808170934\H,0,2.7214509969,
-0.7794918015,2.0174662115\H,0,4.2607821985,-1.4826792351,1.49841071\H
,0,4.2219612941,-0.2389943127,2.7720640567\H,0,5.5848064135,-1.9537361
06,3.6615520647\H,0,-3.1037929235,2.9530277289,4.4926099797\Zn,0,5.296
9967933,-3.3502620908,-5.7144246481\C1,0,4.4214373096,-5.3300449963,6.0
362760978\C1,0,7.1013125857,-2.090139053,5.914732528\\Version=ES64L-G1
6RevA.03\State=1-A\HF=-3467.1113317\RMSD=3.458e-09\PG=C01 [X(C12H16Cl2
O4Zn1)]\@

I2959- ZnCl₂ Toluene

1\1\GINC-R145\SP\RM062X TD-FC\6-31+G(d,p)\C12H16Cl2O4Zn1\ROOT\30-Jan-2

```
019\0\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent
=toluene) td(nstates=10,50-50) guess=read geom=allcheck maxdisk=214748
3648\\title\\0,1\C,0,-3.484262717,2.3972013172,6.3206604373\C,0,-2.168
7410157,1.6898318397,6.5582266656\O,0,-1.814004049,1.0795443594,5.3148
608956\C,0,-0.647590576,0.4151089769,5.223072864\C,0,0.2554844413,0.26
58265061,6.2839454487\H,0,0.0535319486,0.6941077462,7.2577806839\C,0,1
.4273982208,-0.4463911559,6.0794404047\H,0,2.1270687264,-0.5684900625,
6.8990751721\C,0,1.7377009185,-1.0121968647,4.8326388406\C,0,0.8149096
097,-0.8515804644,3.7806583545\H,0,0.9907781041,-1.2850933119,2.804662
5471\C,0,-0.3608786442,-0.1529576301,3.9722553218\H,0,-1.0795855539,-0
.035188386,3.1685733437\C,0,3.0083485675,-1.7523805036,4.7311676111\C,
0,3.5899219626,-2.2630042207,3.3922876673\C,0,2.7845665333,-3.46231401
29,2.8927287018\C,0,3.7445558158,-1.1457985612,2.3613651133\O,0,4.9001
27214,-2.7847152108,3.6713946634\O,0,-3.357743686,3.4275209373,5.36275
69024\O,0,3.6443858909,-1.9839410766,5.7636319871\H,0,-3.8088107771,2.
8663812469,7.2529928123\H,0,-4.2460285325,1.6653192967,6.0195104288\H,
0,-2.2730126142,0.9235505922,7.3357944949\H,0,-1.3950942849,2.41134274
66,6.8464236956\H,0,1.7461358953,-3.2063613746,2.6804796625\H,0,2.7996
378512,-4.2602425614,3.6411124358\H,0,3.2534576591,-3.834631348,1.9783
628644\H,0,2.7879268252,-0.7628144507,2.0091997785\H,0,4.288155188,-1.
5441645557,1.499644025\H,0,4.3084381364,-0.3052291134,2.7811608853\H,0
,5.5795374214,-2.109360935,3.5051694937\H,0,-3.0696520063,3.0292137688
,4.5314294566\Zn,0,5.3331279458,-3.2421796562,5.7493114781\Cl,0,4.6612
229959,-5.2485976423,6.3913920049\Cl,0,7.1755265852,-1.9722762354,5.77
8152857\\Version=ES64L-G16RevA.03\State=1-A\HF=-3467.1431507\RMSD=5.33
4e-09\PG=C01 [X(C12H16Cl2O4Zn1)]\@
```

I2959- ZnCl₂ DCM

```
1\1\GINC-R109\SP\RM062X TD-FC\6-31+G(d,p)\C12H16Cl2O4Zn1\ROOT\30-Jan-2
019\0\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent
=dichloromethane) td(nstates=10,50-50) guess=read geom=allcheck maxdis
k=2147483648\\title\\0,1\C,0,-7.1579046488,-0.993832526,-0.0587653279\
C,0,-5.6733382081,-1.265050298,0.0245453219\O,0,-5.026027116,-0.000123
3374,-0.1521237832\C,0,-3.6842118874,0.0619538802,-0.095214243\C,0,-2.
8550438968,-1.0497802901,0.1092912355\H,0,-3.2687657956,-2.0424678998,
0.2377400873\C,0,-1.4806092485,-0.8703364007,0.1383874142\H,0,-0.83791
12756,-1.7305652898,0.2908990363\C,0,-0.8959824573,0.3946842284,-0.043
3692163\C,0,-1.749082573,1.4994204578,-0.243567372\H,0,-1.3630977655,2
.5019598664,-0.3739001104\C,0,-3.120470558,1.3369024875,-0.2630687337\
H,0,-3.7800613133,2.1853053742,-0.4116285841\C,0,0.574194158,0.4560951
14,-0.0181642614\C,0,1.3675810315,1.6991989481,-0.4576076259\C,0,1.004
1097899,2.138630619,-1.8754381722\C,0,1.247644314,2.8082276864,0.58963
72227\O,0,2.7431801197,1.2688247107,-0.4936298597\O,0,-7.5987158186,-0
.146529299,0.9873194229\O,0,1.2036099847,-0.5428222874,0.3554737415\H,
0,-7.6955203527,-1.9393284058,0.0473388219\H,0,-7.400118684,-0.5654930
546,-1.0402136063\H,0,-5.3629869757,-1.9588958295,-0.7655490435\H,0,-5
.4113835213,-1.6765271903,1.0061580435\H,0,-0.0103514269,2.5305189594,
-1.9445274093\H,0,1.1078294997,1.29758702,-2.5667697618\H,0,1.69875803
12,2.9282080344,-2.1764615116\H,0,0.2314689517,3.1936972984,0.66864158
05\H,0,1.898240962,3.6386740908,0.294976151\H,0,1.5619025375,2.4382804
812,1.5701039869\H,0,3.3302281853,2.0278203724,-0.3455775604\H,0,-7.15
45041047,0.7074921343,0.8913947609\Zn,0,3.2784922965,-0.634715541,0.26
25472213\Cl,0,3.8483421452,-1.9914415478,-1.4403342794\Cl,0,4.25051762
08,-0.1387745666,2.2393334139\\Version=ES64L-G16RevA.03\State=1-A\HF=-
3467.160563\RMSD=1.067e-09\PG=C01 [X(C12H16Cl2O4Zn1)]\@
```

I2959- ZnCl₂ Acetonitrile

```
1\1\GINC-R107\SP\RM062X TD-FC\6-31+G(d,p)\C12H16Cl2O4Zn1\ROOT\30-Jan-2
019\0\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent
=acetonitrile) td(nstates=10,50-50) guess=read geom=allcheck maxdisk=2
147483648\\title\\0,1\C,0,-3.5526458638,2.3289178661,6.3002508368\C,0,
-2.2508057367,1.6066573298,6.5596760399\O,0,-1.8098487146,1.1144200484
,5.2885152581\C,0,-0.6402305289,0.4581495523,5.2101932387\C,0,0.175271
8697,0.1731901955,6.3154012905\H,0,-0.1069333051,0.4807292871,7.314884
1412\C,0,1.358930527,-0.5206121165,6.1184703238\H,0,1.9874305354,-0.74
```

5580901,6.9732518214\C,0,1.761058924,-0.9498446571,4.8413062614\C,0,0.
9275610834,-0.6480463231,3.7440063896\H,0,1.1861981808,-0.9392255406,2
.7345734564\C,0,-0.2522312495,0.0459749582,3.9249781023\H,0,-0.8933857
792,0.2818594531,3.0821885432\C,0,3.0277326024,-1.6879414312,4.7497113
961\C,0,3.5261615628,-2.3281317128,3.4445032637\C,0,2.5365365548,-3.36
01508588,2.9021499236\C,0,3.9289758855,-1.2521255844,2.4339927668\O,0,
4.7137882787,-3.0482980321,3.8229427948\O,0,-3.3763007944,3.440969216,
5.4386302722\O,0,3.7239499521,-1.8079507374,5.7701922476\H,0,-3.936496
3276,2.7144228673,7.2479008257\H,0,-4.2885069594,1.6265443498,5.887575
2924\H,0,-2.4046816939,0.7724427781,7.2536938158\H,0,-1.4998725339,2.2
945616896,6.9649048498\H,0,1.6124359794,-2.908817408,2.5431688455\H,0,
2.2961855908,-4.0912704919,3.6792907297\H,0,3.0132877683,-3.8787288549
,2.0651274856\H,0,3.0777044294,-0.6665506783,2.0883733844\H,0,4.374597
6495,-1.7445483277,1.5633652209\H,0,4.6661245866,-0.5767527119,2.87865
37351\H,0,5.2712115835,-3.199782433,3.0421861768\H,0,-3.060315995,3.11
11886138,4.5863929741\Zn,0,5.5020761396,-2.861751766,5.7805554045\Cl,0
,5.3230322085,-4.9350552497,6.6430094736\Cl,0,7.3885435896,-1.66382238
84,5.4773034179\\Version=ES64L-G16RevA.03\State=1-A\HF=-3467.1630826\R
MSD=2.292e-09\PG=C01 [X(C12H16Cl2O4Zn1)]\@

I2959- ZnCl₂ Water

1\1\GINC-R142\SP\RM062X TD-FC\6-31+G(d,p)\C12H16Cl2O4Zn1\ROOT\30-Jan-2
019\0\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) scrf(smd,solvent
=h2o) td(nstates=10,50-50) guess=read geom=allcheck maxdisk=2147483648
\title\0,1\C,0,-7.0599681145,-1.1522416589,-0.2176730495\C,0,-5.5647
998015,-1.3454002211,-0.1423065027\O,0,-4.9741096135,-0.0449068946,-0.
2551344397\C,0,-3.6300165979,0.0646169421,-0.1697791729\C,0,-2.7674760
308,-1.0236603229,0.016081217\H,0,-3.1466051557,-2.0344631946,0.101682
0636\C,0,-1.4014342529,-0.7951768694,0.0862447191\H,0,-0.7347061252,-1
.6382895806,0.2289588747\C,0,-0.8589913063,0.496168804,-0.0226757574\C
,0,-1.7462002874,1.5740778281,-0.2141997213\H,0,-1.3939527915,2.591519
1906,-0.3212890971\C,0,-3.1103090744,1.3620694857,-0.285649896\H,0,-3.
794376232,2.1905729888,-0.4352705363\C,0,0.6108675417,0.6141937323,0.0
523927244\C,0,1.3505570715,1.9654109045,0.0030140392\C,0,1.2132908335,
2.5898491234,-1.3842878472\C,0,0.9292509793,2.886470951,1.1470524208\O
,0,2.756637814,1.6989477352,0.1620117484\O,0,-7.557946388,-0.416295632
9,0.8927703315\O,0,1.2836765262,-0.419258121,0.1416822784\H,0,-7.54070
73813,-2.1325764583,-0.1921946652\H,0,-7.3255074672,-0.6561384513,-1.1
586010756\H,0,-5.2198202511,-1.9824196447,-0.9644743819\H,0,-5.2830895
672,-1.7933306351,0.8169709018\H,0,0.1777175634,2.8147544937,-1.638274
7178\H,0,1.6174686166,1.906348938,-2.1371925816\H,0,1.7900815118,3.518
095124,-1.3993932422\H,0,-0.1039802102,3.2176230888,1.0634692952\H,0,1
.574669614,3.7693808611,1.1277009935\H,0,1.0528243432,2.3734591743,2.1
065195469\H,0,3.0257390128,1.9162175513,1.0692123246\H,0,-7.2109218651
,0.4849574511,0.8390966133\Zn,0,3.4022343965,-0.3371707688,-0.04576535
4\Cl,0,3.8740884647,-1.6447696595,-1.9029788204\Cl,0,4.1116802241,-1.4
141922543,1.8826057662\\Version=ES64L-G16RevA.03\State=1-A\HF=-3467.16
7073\RMSD=2.370e-09\PG=C01 [X(C12H16Cl2O4Zn1)]\@

I2959-Ethene Gas

Ortho-

1\1\GINC-R1457\SP\RM062X TD-FC\6-31+G(d,p)\C14H18O4\ROOT\08-Dec-2018\
\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50)
guess=read geom=allcheck maxdisk=2147483648\\title\0,1\C,0,-1.0011103
191,2.2790480629,-2.8070517005\C,0,0.1689634633,1.4243597797,-2.365761
024\O,0,-0.0945211461,1.0703168449,-1.0125295203\C,0,0.7614343744,0.23
3603763,-0.3761046939\C,0,1.9220855816,-0.2788410378,-0.9509671425\C,0
,2.7587622754,-1.1491460746,-0.2376295458\C,0,2.4392676436,-1.46763863
36,1.1013540001\C,0,1.2765297095,-0.9165025433,1.66534281\H,0,1.005034
6274,-1.1559754797,2.6853133716\C,0,0.434494354,-0.0913199289,0.945029
2199\H,0,-0.4676288576,0.3212520497,1.3827503242\C,0,3.2998493175,-2.4
120791772,1.869781128\C,0,3.4385609239,-2.3553720709,3.4142438609\C,0,
3.5683810212,-0.9325504325,3.9532777606\C,0,2.2855370291,-3.1324573183
,4.0712491672\O,0,4.646040596,-3.0112598809,3.7457388568\O,0,-2.211461
4758,1.5586390438,-2.7591117151\O,0,3.9495893241,-3.2680620906,1.29154

65311\H,0,-0.8543381896,2.5872215929,-3.8453185157\H,0,-1.0478517381,3
.1807230695,-2.1808879984\H,0,1.1122790175,1.9816143611,-2.4351721918\
H,0,0.2283076431,0.5173279855,-2.9803125471\H,0,2.6400164838,-0.364253
582,3.8811358956\H,0,4.3535781424,-0.3943784921,3.415244219\H,0,3.8598
500191,-0.9987660208,5.0048225042\H,0,1.3063364734,-2.668373997,3.9358
147331\H,0,2.4967976271,-3.1949552764,5.1420960369\H,0,2.2485779879,-4
.1489325461,3.6687816107\H,0,4.842529752,-3.6297992518,3.024549077\H,0
, -2.3247903622,1.2319601744,-1.8578312379\H,0,2.2174133227,0.008316355
3,-1.9524728413\C,0,3.9771481002,-1.6475693507,-0.9153177253\C,0,4.033
6901053,-1.9379841756,-2.2168244727\H,0,4.8614004381,-1.7873631247,-0.
301794874\H,0,3.1577423637,-1.8832126259,-2.8576242504\H,0,4.957814371
4,-2.2786499714,-2.6703091101\\Version=ES64L-G16RevA.03\State=1-A\HF=-
844.8764625\RMSD=3.710e-09\PG=C01 [X(C14H18O4)]\@

Meta-

1\1\GINC-R2395\SP\RM062X TD-FC\6-31+G(d,p)\C14H18O4\ROOT\08-Dec-2018\
\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50)
guess=read geom=allcheck maxdisk=2147483648\\title\\0,1\C,0,-0.2774187
605,1.2964341154,-2.9314030439\C,0,0.947411758,0.5562391945,-2.4323525
109\O,0,0.8313432334,0.5548750495,-1.0125111943\C,0,1.6507934722,-0.22
43243504,-0.2724746223\C,0,1.3394892195,-0.3491590215,1.0997058039\C,0
,2.1593912151,-1.1717843327,1.8760388205\C,0,3.2700822146,-1.843483875
1,1.3547492439\C,0,3.5541124131,-1.6839240184,-0.0063536233\H,0,4.4143
111905,-2.198129839,-0.4209524032\C,0,2.7550076659,-0.8892103002,-0.81
46887907\H,0,2.9968593229,-0.7846874827,-1.8651914747\C,0,4.1888461507
, -2.7280298424,2.1338664692\C,0,4.0216560181,-3.0094164112,3.643224804
4\C,0,4.1713735772,-1.7230516118,4.465577531\C,0,2.7024829726,-3.74106
5693,3.9235892192\O,0,5.0652413989,-3.8740013391,4.037470268\O,0,-1.46
24226202,0.6307090959,-2.5616123592\O,0,5.1262830172,-3.2646626172,1.5
643276434\H,0,-0.2600176792,1.3376874913,-4.02337977\H,0,-0.2597381325
,2.326191007,-2.546571441\H,0,1.8720680765,1.0615294626,-2.7387644471\
H,0,0.9446217119,-0.4758823663,-2.8028873529\H,0,3.357884951,-1.011426
8875,4.3166525394\H,0,5.1172678994,-1.2327751113,4.2194708415\H,0,4.20
14511383,-2.0074287075,5.5207035058\H,0,1.8165125286,-3.1303627101,3.7
429860917\H,0,2.7109799787,-4.0471100831,4.9730241851\H,0,2.6398699815
, -4.6425091333,3.3078222818\H,0,5.5986896912,-4.0609134292,3.247895192
6\H,0,-1.4515123881,0.5106155872,-1.6026362169\C,0,0.1969545006,0.3034
248421,1.7618326529\C,0,-0.578333813,1.3098190541,1.3393024567\H,0,-0.
0070874277,-0.0996432086,2.7534833524\H,0,-0.4376269488,1.8037311352,0
.3869562334\H,0,1.8979630659,-1.2708009756,2.9224186137\H,0,-1.3704125
934,1.6765183126,1.9837095001\\Version=ES64L-G16RevA.03\State=1-A\HF=-
844.8812172\RMSD=1.528e-09\PG=C01 [X(C14H18O4)]\@

I2959-Butene Gas

Ortho-

1\1\GINC-R3326\SP\RM062X TD-FC\6-31+G(d,p)\C16H20O4\ROOT\08-Dec-2018\
\#\ M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50)
guess=read geom=allcheck maxdisk=2684354560\\title\\0,1\C,0,-1.0264562
097,2.3084994518,-2.7844241527\C,0,0.1458658321,1.4541410174,-2.348488
7111\O,0,-0.1173774144,1.089274544,-0.9981491509\C,0,0.7401680828,0.24
97290992,-0.3674725634\C,0,1.9021355049,-0.2546388633,-0.9449352248\C,
0,2.7428731003,-1.128886707,-0.237837781\C,0,2.4216007245,-1.457382466
2,1.0998231217\C,0,1.2577075553,-0.9116452247,1.6665174614\H,0,0.98669
30272,-1.1584395084,2.6848433737\C,0,0.4131144448,-0.084607052,0.95169
32028\H,0,-0.490218262,0.3226368234,1.3918018855\C,0,3.2787293651,-2.4
070604862,1.8652678147\C,0,3.4177011396,-2.3542315137,3.4103189288\C,0
,3.5466248181,-0.9331514905,3.9538957722\C,0,2.2660177014,-3.134723043
6,4.0656857504\O,0,4.6262937014,-3.0096419195,3.7391875031\O,0,-2.2346
172771,1.5840480715,-2.7430165671\O,0,3.9248553911,-3.2655869557,1.286
3552153\H,0,-0.8796803467,2.6249319181,-3.8201945885\H,0,-1.076492876,
3.2053326882,-2.1516070904\H,0,1.0874979894,2.0148126081,-2.4132666241
\H,0,0.2083121913,0.5517537292,-2.9696116331\H,0,2.6175018271,-0.36574
93722,3.8848621981\H,0,4.3304414818,-0.3921728949,3.4166802152\H,0,3.8
394409944,-1.0025298108,5.0048641776\H,0,1.2862331594,-2.6710462761,3.

9330671136\H,0,2.4785047845,-3.2008644537,5.1360700861\H,0,2.229423124
9,-4.1497496861,3.6595150738\H,0,4.8187756727,-3.6314920566,3.01981390
41\H,0,-2.3485272892,1.2514872936,-1.8439725048\H,0,2.1969947803,0.045
9698881,-1.9424741008\C,0,3.9593233694,-1.6185501863,-0.911272766\C,0,
4.04207019,-1.8624216053,-2.2295908816\H,0,4.8316915071,-1.806892548,-
0.2924182723\H,0,3.1615790162,-1.7578513778,-2.8638335197\C,0,5.264492
5838,-2.315557112,-2.8811438242\C,0,5.3543522785,-2.5784386271,-4.1902
632887\H,0,6.1376951687,-2.4411539996,-2.2425628936\H,0,4.4956817642,-
2.4651884494,-4.8471608835\H,0,6.281877403,-2.9152334457,-4.6395157759
\Version=ES64L-G16RevA.03\State=1-A\HF=-922.2491674\RMSD=5.280e-09\PG
=C01 [X(C16H2004)]\@

Meta-

1\1\GINC-R2769\SP\RM062X TD-FC\6-31+G(d,p)\C16H2004\ROOT\08-Dec-2018\
\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50)
guess=read geom=allcheck maxdisk=2684354560\title\0,1\C,0,1.78598885
8,1.6078176258,-3.5261674964\C,0,1.3203226052,0.2054108683,-3.85963183
94\O,0,-0.0041022962,0.1063976064,-3.3466104002\C,0,-0.6563497691,-1.0
788690643,-3.4217654855\C,0,-1.9475416952,-1.1075619859,-2.8528374211\
C,0,-2.6633368067,-2.303121924,-2.9074363597\C,0,-2.1318628546,-3.4633
489666,-3.482151703\C,0,-0.8464523026,-3.400672966,-4.0332217639\H,0,-
0.4339216306,-4.2947817817,-4.4878155605\C,0,-0.1118989859,-2.22303047
83,-4.011012248\H,0,0.8789507797,-2.204333291,-4.4476563135\C,0,-2.838
2069551,-4.7770512027,-3.5731662042\C,0,-4.2414270844,-5.0297845483,-2
.9786949327\C,0,-4.2554387098,-4.8111218507,-1.460899735\C,0,-5.300084
1338,-4.1899052159,-3.7068385048\O,0,-4.5622707948,-6.3868193645,-3.19
74833705\O,0,1.8247371063,1.8179323993,-2.1333488103\O,0,-2.2938433035
, -5.7114808933,-4.1403600543\H,0,1.1293402903,2.3358606908,-4.02251453
66\H,0,2.8033123875,1.7510196361,-3.8989628877\H,0,1.9630159918,-0.533
2892076,-3.3652602554\H,0,1.320791736,0.0336449829,-4.9437854692\H,0,-
4.1290927974,-3.767094866,-1.1696403063\H,0,-3.4675156958,-5.405943434
2,-0.9908437842\H,0,-5.2186536364,-5.1666792016,-1.0856062342\H,0,-5.2
013985964,-3.1165341144,-3.5365849337\H,0,-6.2815193503,-4.5141269534,
-3.3507798801\H,0,-5.2492565413,-4.3813907384,-4.7822670497\H,0,-3.835
4476644,-6.775464638,-3.7109893084\H,0,0.9481535559,1.6232403729,-1.77
81432722\C,0,-2.5050987194,0.1071081183,-2.2426802967\C,0,-3.419172525
6,0.1220553117,-1.2575518236\H,0,-2.1296857314,1.0541335374,-2.6248074
62\H,0,-3.7687155244,-0.8140464745,-0.8204984767\C,0,-3.9776925189,1.3
472784895,-0.7005561627\C,0,-4.880319917,1.3700208226,0.2872492413\H,0
, -3.6238872357,2.2832020722,-1.1312537256\H,0,-5.2500601939,0.45015136
19,0.7328692494\H,0,-3.6688059036,-2.2951532403,-2.5079597234\H,0,-5.2
733074364,2.3026915054,0.6760533008\Version=ES64L-G16RevA.03\State=1-
A\HF=-922.2547902\RMSD=5.293e-09\PG=C01 [X(C16H2004)]\@

I2959-Hexene Gas

Ortho-

1\1\GINC-R1188\SP\RM062X TD-FC\6-31+G(d,p)\C18H2204\ROOT\11-Dec-2018\
\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50)
guess=read geom=allcheck maxdisk=2684354560\title\0,1\C,0,-1.0765227
15,2.3491735229,-2.7211879579\C,0,0.0979305456,1.4911523313,-2.2983361
148\O,0,-0.1590780751,1.1134184818,-0.9504518813\C,0,0.7018822489,0.26
83807241,-0.3315878091\C,0,1.8618739073,-0.2288242563,-0.9184011265\C,
0,2.7072885794,-1.1090514438,-0.223108086\C,0,2.390849421,-1.450416470
4,1.1129213378\C,0,1.2289249751,-0.9110146219,1.6894627135\H,0,0.96241
30832,-1.1678997815,2.7065384218\C,0,0.3802190409,-0.07867885,0.985784
3894\H,0,-0.5218588391,0.3233390356,1.4331765893\C,0,3.2496310486,-2.4
077161632,1.8669113867\C,0,3.403107306,-2.3605089994,3.410766037\C,0,3
.5360564349,-0.9415583795,3.9585251075\C,0,2.2581238996,-3.1441273974,
4.0740563357\O,0,4.6155040078,-3.0160758422,3.7254845092\O,0,-2.284237
7428,1.6238156294,-2.6822982797\O,0,3.8859398344,-3.2678779444,1.27960
05244\H,0,-0.9338702766,2.6757927882,-3.7543598396\H,0,-1.1244986742,3
.2397268469,-2.0794184378\H,0,1.039090028,2.0527763447,-2.3621550659\H
,0,0.1578891524,0.594687777,-2.9282688831\H,0,2.6057813159,-0.37489888
19,3.8992747028\H,0,4.3145892703,-0.3978907762,3.4163688383\H,0,3.8379

108177,-1.0143689929,5.006697618\H,0,1.2770691522,-2.6800476321,3.9526
964158\H,0,2.4807916976,-3.214419505,5.1421004226\H,0,2.2177019271,-4.
1574930581,3.6640897786\H,0,4.7970661864,-3.6413862195,3.0063621784\H,
0,-2.3947160471,1.2826863486,-1.786050733\H,0,2.1524514163,0.083670658
, -1.9135109955\C,0,3.9216145908,-1.5899967171,-0.9030132301\C,0,4.0094
799433,-1.8020833157,-2.2287529774\H,0,4.7896070969,-1.8012264913,-0.2
857465989\H,0,3.1313456686,-1.6753198989,-2.8620472583\C,0,5.225191808
, -2.2439594349,-2.8848720121\C,0,5.3198129624,-2.4759170673,-4.2085407
855\H,0,6.1014145618,-2.3931517016,-2.2536843898\H,0,4.4426385445,-2.3
308195897,-4.8402647147\C,0,6.5395058448,-2.9178739468,-4.866916295\C,
0,6.6361002578,-3.1476173517,-6.1827067224\H,0,7.4106068531,-3.0640552
834,-4.2292518702\H,0,5.7824323472,-3.0109650369,-6.8415052298\H,0,7.5
645065942,-3.4779294376,-6.634910012\Version=ES64L-G16RevA.03\State=1
-A\HF=-999.6225889\RMSD=5.428e-09\PG=C01 [X(C18H22O4)]\@

Meta-

1\1\GINC-R1198\SP\RM062X TD-FC\6-31+G(d,p)\C18H22O4\ROOT\11-Dec-2018\
\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50)
guess=read geom=allcheck maxdisk=2684354560\title\0,1\C,0,1.72066258
51,1.6082260198,-4.3414496049\C,0,1.224585547,0.1935245918,-4.55902637
91\O,0,0.0248058883,0.0839303184,-3.8017312344\C,0,-0.6080591871,-1.11
23759508,-3.7317492739\C,0,-1.7709316906,-1.1498703022,-2.9270685904\C
,0,-2.4519500189,-2.3592753033,-2.8302612548\C,0,-2.0154456634,-3.5245
781552,-3.4766215833\C,0,-0.8612829764,-3.4533117012,-4.261584269\H,0,
-0.4839665841,-4.3194987584,-4.7884082122\C,0,-0.1625371901,-2.2563123
045,-4.3937961219\H,0,0.7273240954,-2.2291101431,-5.0101346939\C,0,-2.
8473062387,-4.7502291333,-3.2756088877\C,0,-2.5245353682,-6.1126957323
, -3.9283416888\C,0,-2.5964242989,-6.0234034903,-5.4581483158\C,0,-1.18
00583563,-6.6585223788,-3.4300410123\O,0,-3.5173279286,-7.0300559346,-
3.5223928542\O,0,2.0258762157,1.8422297178,-2.9860332586\O,0,-3.835997
7265,-4.6930178403,-2.5612319401\H,0,0.9667419507,2.3176011918,-4.7102
850713\H,0,2.6433378606,1.760829032,-4.9070587142\H,0,1.9634377066,-0.
5264355382,-4.1858600914\H,0,1.0215707695,0.0025372533,-5.6208984253\H
,0,-1.8069479504,-5.4116949816,-5.8974062048\H,0,-3.5657436744,-5.6179
385152,-5.7611756683\H,0,-2.5154693393,-7.0397390594,-5.8527324741\H,0
, -0.3202910808,-6.0780348587,-3.768055582\H,0,-1.0813495889,-7.6823860
321,-3.8003833563\H,0,-1.1748604085,-6.6911786873,-2.3370365541\H,0,-4
.1312297541,-6.5521870516,-2.9410325584\H,0,1.2383206988,1.6424566479,
-2.463824924\C,0,-2.2243738561,0.0691346496,-2.2469447676\C,0,-2.99696
24287,0.0953388902,-1.1447877661\H,0,-1.8930360145,1.0116516002,-2.676
952596\H,0,-3.3016531537,-0.8370266311,-0.6698698901\C,0,-3.4505654184
, 1.3218975106,-0.5189030347\C,0,-4.2180209738,1.3584472531,0.588027742
3\H,0,-3.1450175573,2.2590584025,-0.9853813379\H,0,-4.5264844983,0.422
1719898,1.0542881569\C,0,-4.6743297308,2.5892000251,1.2150011666\C,0,-
5.4386512704,2.6268174269,2.3140526915\H,0,-4.3622217913,3.5205628664,
0.7437176112\H,0,-5.7642636865,1.7127598801,2.803734254\H,0,-5.7581708
669,3.5659648393,2.751662148\H,0,-3.3690130469,-2.4159186233,-2.253251
5785\Version=ES64L-G16RevA.03\State=1-A\HF=-999.6279288\RMSD=5.953e-0
9\PG=C01 [X(C18H22O4)]\@

I2959-Phenyl Gas

Ortho-

1\1\GINC-R3059\SP\RM062X TD-FC\6-31+G(d,p)\C18H20O4\ROOT\08-Dec-2018\
\#\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50)
guess=read geom=allcheck maxdisk=2684354560\title\0,1\C,0,-1.3852009
359,1.7386865724,-2.799124554\C,0,-0.0895247702,1.0446961426,-2.432848
9181\O,0,-0.1239428439,0.8720292703,-1.0223314158\C,0,0.8911917808,0.1
953915363,-0.4225999651\C,0,2.0002930539,-0.307089902,-1.1026881802\C,
0,3.003640299,-0.9930646734,-0.4056831301\C,0,2.8857296251,-1.17937964
43,0.9754599022\C,0,1.7847078897,-0.6358429814,1.6507889137\H,0,1.7088
83956,-0.766281064,2.7261907884\C,0,0.7900671107,0.0397807916,0.964138
1891\H,0,-0.069956859,0.4565269325,1.4769193079\C,0,3.8368348035,-1.99
64916964,1.8044772623\C,0,3.936147604,-3.5394159139,1.6383338779\C,0,2
.735169411,-4.1319997582,0.9162938864\C,0,5.2510276239,-3.9369553453,0

.9560105768\O,0,3.919442611,-4.0698219086,2.955463958\O,0,-2.503360896
9,0.9462488859,-2.4693733151\O,0,4.4401976521,-1.4869830136,2.72881700
16\H,0,-1.4177688653,1.9025523525,-3.8792381351\H,0,-1.4269723023,2.71
57525749,-2.2982718676\H,0,0.7778875491,1.6534799845,-2.720967128\H,0,
-0.0334399719,0.065510645,-2.9256081051\H,0,2.7016719574,-3.8034933393
, -0.1260525499\H,0,1.8040247134,-3.8420285663,1.4105212527\H,0,2.81730
06263,-5.2218590733,0.9408461492\H,0,5.2556181466,-3.7065668098,-0.111
8614847\H,0,5.3705989014,-5.0159373402,1.0880809022\H,0,6.0971715047,-
3.4296385426,1.430754981\H,0,4.4850734574,-3.5023215482,3.4996042075\H
,0,-2.4528819824,0.745226459,-1.5264725095\H,0,2.1280231753,-0.1459778
989,-2.167140354\C,0,4.2127567546,-1.4522489146,-1.1358889091\C,0,4.10
53856657,-2.2685524267,-2.2678568341\H,0,3.1214373093,-2.5800019121,-2
.609488114\C,0,5.2491942714,-2.7078831231,-2.9305254798\H,0,5.15584673
84,-3.3559726684,-3.7962674321\C,0,6.5115185891,-2.3222109475,-2.47833
61813\H,0,7.4020428744,-2.6660930796,-2.9946544046\C,0,6.6252980734,-1
.4927685606,-1.3637010007\H,0,7.6045252865,-1.1838427568,-1.0119300601
\C,0,5.482837347,-1.0622344094,-0.6933464586\H,0,5.5691160657,-0.41733
23292,0.1772623297\Version=ES64L-G16RevA.03\State=1-A\HF=-998.4812396
\RMSD=3.842e-09\PG=C01 [X(C18H2004)]\@

Meta-

1\1\GINC-R2370\SP\RM062X TD-FC\6-31+G(d,p)\C18H2004\ROOT\08-Dec-2018\O
\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50)
guess=read geom=allcheck maxdisk=2684354560\title\0,1\C,0,-1.4096748
513,2.2234760955,-2.4293476401\C,0,-0.1096403369,1.4631019172,-2.25023
62799\O,0,-0.0754343977,1.1053770467,-0.8743344265\C,0,0.8963483373,0.
2835580232,-0.4150566518\C,0,0.7332515904,-0.2104749132,0.898815105\C,
0,1.7104624376,-1.061996909,1.3978251499\H,0,1.6155932947,-1.446494539
5,2.4086286024\C,0,2.8374396855,-1.4409228699,0.650825399\C,0,2.968303
6778,-0.9369612777,-0.6449502101\H,0,3.8154900072,-1.1945496021,-1.266
6188896\C,0,2.0059314734,-0.0838756915,-1.1775179471\H,0,2.127169312,0
.2886667805,-2.1873168639\C,0,3.8054960855,-2.3604173564,1.3216881617\C
0,5.1160089264,-2.8427263718,0.6608993178\C,0,4.8241709048,-3.702121
8399,-0.5764072406\C,0,6.0489260654,-1.6642165139,0.3555295677\O,0,5.7
864983382,-3.6681950485,1.5887065058\O,0,-2.5194775668,1.4274371864,-2
.089182266\O,0,3.5679106889,-2.7615600748,2.4502482747\H,0,-1.52549818
51,2.5072188336,-3.4785434585\H,0,-1.3758843055,3.1408704076,-1.824537
9176\H,0,0.7530099703,2.0920082209,-2.5064722323\H,0,-0.1050346248,0.5
552041959,-2.8663172157\H,0,4.3848701228,-3.1427228421,-1.403849789\H,
0,4.1509273555,-4.521150871,-0.308739391\H,0,5.771070561,-4.1361632192
, -0.908265859\H,0,5.6754529434,-1.0044976669,-0.4290580005\H,0,7.01105
01456,-2.0768180553,0.040591089\H,0,6.212661652,-1.0753929707,1.262254
1834\H,0,5.2282240414,-3.7224656171,2.3815242487\H,0,-2.4057045135,1.1
355603223,-1.1745069783\C,0,-0.4586065927,0.1299293362,1.7204179948\C,
0,-0.9163383445,1.448757262,1.8441669684\H,0,-0.4002919515,2.244664299
8,1.3175611286\C,0,-2.0150842892,1.7436840765,2.6464766768\H,0,-2.3520
721096,2.7715080205,2.7388689858\C,0,-2.6779747198,0.7269294811,3.3335
85192\H,0,-3.5365305099,0.9585263934,3.9558475565\C,0,-2.2316344449,-0
.587430638,3.2161888294\H,0,-2.7431305903,-1.3866315852,3.7432335499\C
,0,-1.1302884104,-0.8828605526,2.4156854445\H,0,-0.7940418723,-1.91099
08728,2.3145183255\Version=ES64L-G16RevA.03\State=1-A\HF=-998.4852174
\RMSD=7.765e-09\PG=C01 [X(C18H2004)]\@

I2959-Phenyl (fused) Gas

1\1\GINC-R929\SP\RM062X TD-FC\6-31+G(d,p)\C16H1804\ROOT\11-Dec-2018\O\
\# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50) g
uess=read geom=allcheck maxdisk=2684354560\title\0,1\C,0,-1.49074337
43,2.1623885237,-2.39498373\C,0,-0.1319909048,1.4959308691,-2.34030915
04\O,0,0.0194355066,1.0224872886,-1.0068632524\C,0,1.1244797489,0.3071
034874,-0.6917901509\C,0,1.1920654342,-0.1489892292,0.6647234377\C,0,0
.1398496544,0.1438359307,1.5684805509\C,0,2.3219997454,-0.9006648718,1
.097494707\C,0,2.3300821043,-1.3599556715,2.4437806875\C,0,3.368643786
7,-1.1955390506,0.148581876\C,0,3.2353793221,-0.7478860121,-1.14705037
32\H,0,4.0110620512,-0.95508515,-1.8732723135\C,0,2.1310802385,0.01407

33348,-1.5816750255\H,0,2.0974982375,0.3554777525,-2.6081747079\C,0,4.6038926253,-1.9211710286,0.5646467468\C,0,5.3717067578,-2.8806814161,-0.3870002375\C,0,4.4521612142,-3.7436957788,-1.2462493958\C,0,6.3876053979,-2.0876288986,-1.2266275605\O,0,6.0961909125,-3.7766223972,0.4331704793\O,0,-2.5271571296,1.2392731055,-2.1487526177\O,0,5.0592803101,-1.7922740881,1.689467779\H,0,-1.6564083617,2.5661423382,-3.3970132003\H,0,-1.516730395,2.9941627938,-1.6775381763\H,0,0.6696634131,2.2067046064,-2.5798380545\H,0,-0.0989470269,0.6497436744,-3.0377995543\H,0,3.942789636,-3.1718500395,-2.0232329967\H,0,3.7010278396,-4.2356094411,-0.6222952362\H,0,5.0633199137,-4.516687336,-1.7196077654\H,0,5.9292539097,-1.4259137289,-1.9647750775\H,0,7.0169743392,-2.8110799296,-1.7518189311\H,0,7.0257975896,-1.4895501676,-0.5695367095\H,0,6.2737719436,-3.317917142,1.269144461\H,0,-2.3611250335,0.8253665134,-1.2926616679\C,0,0.1877984387,-0.3073930106,2.8639346083\C,0,1.2913270362,-1.0730548622,3.2971312917\H,0,-0.7004407223,0.730988339,1.217229565\H,0,3.1731040355,-1.9340235391,2.8017376906\H,0,-0.6204426858,-0.0803955774,3.5515439423\H,0,1.3243174915,-1.4391201908,4.3184230615\\Version=ES64L-G16RevA.03\State=1-A\HF=-921.0972913\RMSD=2.568e-09\PG=C01 [X(C18H18O4)]\@

I2959-Antiaromatic (fused) Gas

1\1\GINC-R399\SP\RM062X TD-FC\6-31+G(d,p)\C18H18O4\ROOT\11-Dec-2018\0\ \# M062X/6-31+G** scf=tight int(grid=ultrafine) td(nstates=10,50-50) guess=read geom=allcheck maxdisk=2684354560\\title\\0,1\C,-1.6717261952,2.2980603929,-2.3445135293\C,-0.3456534555,1.5685192476,-2.2826937395\O,-0.1711974328,1.2044323321,-0.9172192166\C,0.8859738387,0.4298606085,-0.5748470378\C,0.9853641673,0.0643944988,0.7571634585\C,2.0496923563,-0.7436470969,1.2175955901\C,3.0323836241,-1.2046351534,0.3326475894\C,2.9076261851,-0.8201918523,-1.0196043519\H,3.6457173445,-1.1384013742,-1.7434019344\C,1.8729134857,-0.0170027664,-1.4730682391\H,1.8376666435,0.2586710107,-2.5199452932\C,4.1497590591,-2.0494440994,0.8429068224\C,5.0156902537,-2.9500040285,-0.0716582118\C,4.1764437332,-3.8205258858,-1.0078100098\C,6.0474503771,-2.093389552,-0.8244234352\O,5.7272027803,-3.8393729393,0.763248321\O,-2.7362589091,1.4562102444,-1.9640946301\O,4.4120689669,-2.0597942179,2.0360186875\H,-1.8667009723,2.6155877806,-3.371935303\H,-1.6223093068,3.1923508773,-1.7078273267\H,0.4790240221,2.2141959612,-2.6114263725\H,-0.3833564941,0.665985334,-2.9052171171\H,3.6805647275,-3.2510163413,-1.7947977044\H,3.420035423,-4.3659124629,-0.4370458594\H,4.8456444438,-4.5510391047,-1.4699659439\H,5.607101484,-1.4075765486,-1.5506477698\H,6.7220224527,-2.7748323906,-1.3495623694\H,6.6371130077,-1.5133025704,-0.1088087994\H,5.7007879414,-3.4732427955,1.661693827\H,-2.5276402981,1.0895870132,-1.0953056134\C,0.1347618194,0.3591025509,1.9102463399\C,0.7353908354,-0.3232014194,3.0616776279\C,1.8561529287,-0.9736745493,2.6836345182\C,-0.9683850646,1.0157742129,2.3257391974\C,-1.1137952188,0.7619153378,3.789158862\C,-0.1081481824,-0.0303310349,4.2289514567\H,2.5322286065,-1.5587773433,3.2902392602\H,0.0505570625,-0.3811894598,5.2392696075\H,-1.9172910173,1.1648564152,4.3936131412\H,-1.6399780232,1.629497169,1.7380815009\\Version=ES64L-G16RevA.03\State=1-A\HF=-997.2227382\RMSD=2.492e-09\PG=C01 [X(C18H18O4)]\@