

Can Electrostatic Catalysis of Diels-Alder Reactions be Harnessed with pH-Switchable Charged Functional Groups?

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Table of Contents

Table S1: Kinetic and thermodynamic parameters R=COOH	2
Table S2: Kinetic and thermodynamic parameters R=COO ⁻	3
Table S3: Kinetic and thermodynamic parameters R=NMe ₂	4
Table S4: Kinetic and thermodynamic parameters R=NMe ₂ H ⁺	5
Table S5: pH-switch between neutral (R=COOH) and deprotonated (R=COO ⁻) species	6
Table S6: pH-switch between neutral (R=NMe ₂) and protonated (R=NMe ₂ H ⁺) species	7
Table S7: Distortion/Interaction analysis and transition state bond lengths R=COOH.....	8
Table S8: Distortion/Interaction analysis and transition state bond lengths R=COO ⁻	9
Table S9: Distortion/Interaction analysis and transition state bond lengths R=NMe ₂	10
Table S10: Distortion/Interaction analysis and transition state bond lengths R=NMe ₂ H ⁺	11
Table S11: Solvent dependence of the pH-switch ($\Delta\Delta G^\ddagger$)	12
Figure S1: pi-pi* energies (eV) for both Normal and Inverse Electron demand reactivity	13
Table S12: pi-pi* energies (eV) for both Normal and Inverse Electron demand reactivity	13
Table S13: Components of the G3(MP2)-CC calculation for starting materials	14
Table S14: Components of the G3(MP2)-CC calculation for products.....	14
Table S15: Components of the G3(MP2)-CC calculation for transition states	17
Gaussian Archive Entries	20

Table S1: Kinetic and thermodynamic parameters (kJ mol⁻¹) and the imaginary frequency for each transition state, calculated at M062X/6-31+G** (M06) and G3(MP2)-CC (G3) where R=COOH

T=298.15K	$\Delta E^{\ddagger}_{M06}$	$\Delta H^{\ddagger}_{M06}$	ΔH_{M06}	$\Delta G^{\ddagger}_{M06}$	ΔG^{\ddagger}_{G3}	ΔG_{M06}	$\Delta S^{\ddagger}_{M06}$	ΔS_{M06}	iFreq_{M06}
a	67.3	71.5	-106.0	130.3	121.3	-43.1	-197.8	-209.3	-506.3
b	70.8	74.8	-105.1	137.4	128.6	-41.7	-210.3	-212.9	-518.0
c	80.9	85.4	-102.1	142.9	134.9	-40.2	-193.6	-207.7	-512.4
d	81.2	86.1	-109.4	145.3	138.7	-46.8	-199.0	-212.9	-530.2
T=298.15K	$\Delta E^{\ddagger}_{M06}$	$\Delta H^{\ddagger}_{M06}$	ΔH_{M06}	$\Delta G^{\ddagger}_{M06}$	ΔG^{\ddagger}_{G3}	ΔG_{M06}	$\Delta S^{\ddagger}_{M06}$	ΔS_{M06}	iFreq_{M06}
a	85.0	89.4	-73.7	147.4	138.1	-9.5	-177.3	-194.7	-533.9
b	90.6	94.9	-90.0	151.6	143.6	-27.7	-172.6	-195.1	-470.0
c	94.6	99.4	-72.4	157.0	148.4	-8.2	-175.8	-195.2	-529.2
d	93.4	98.2	-90.0	155.5	147.3	-27.9	-174.8	-194.4	-528.4
T=298.15K	$\Delta E^{\ddagger}_{M06}$	$\Delta H^{\ddagger}_{M06}$	ΔH_{M06}	$\Delta G^{\ddagger}_{M06}$	ΔG^{\ddagger}_{G3}	ΔG_{M06}	$\Delta S^{\ddagger}_{M06}$	ΔS_{M06}	iFreq_{M06}
a	73.7	76.4	-112.5	137.1	129.4	-48.2	-167.8	-181.2	-532.1
b	73.9	76.7	-114.7	141.2	149.2	-50.3	-180.5	-182.8	-542.3
c	68.3	71.2	-119.0	133.9	126.5	-53.4	-174.5	-183.1	-530.7
d	79.0	81.5	-115.2	147.9	140.9	-49.8	-186.8	-184.2	-545.0
T=298.15K	$\Delta E^{\ddagger}_{M06}$	$\Delta H^{\ddagger}_{M06}$	ΔH_{M06}	$\Delta G^{\ddagger}_{M06}$	ΔG^{\ddagger}_{G3}	ΔG_{M06}	$\Delta S^{\ddagger}_{M06}$	ΔS_{M06}	iFreq_{M06}
a	91.5	97.7	-84.3	156.2	147.9	-18.6	-152.1	-167.8	-557.2
b	94.5	94.8	-96.2	153.3	149.2	-32.6	-144.2	-165.8	-509.2
c	90.9	93.8	-84.3	156.7	145.8	-18.5	-145.6	-168.6	-559.1
d	92.4	95.8	-95.7	154.9	148.3	-32.2	-144.3	-165.5	-562.1
e	83.9	87.5	-87.6	151.1	142.6	-22.7	-159.6	-169.7	-538.0
f	87.2	90.8	-96.6	152.2	146.2	-33.2	-156.2	-165.6	-550.3
g	85.1	88.7	-86.9	157.4	143.4	-21.3	-159.2	-170.0	-551.6
h	91.5	94.9	-96.3	153.4	150.2	-33.5	-155.6	-166.1	-563.7

Table S2: Kinetic and thermodynamic parameters (kJ mol⁻¹) and the imaginary frequency for each transition state, calculated at M062X/6-31+G** (M06) and G3(MP2)-CC (G3) where R=COO⁻

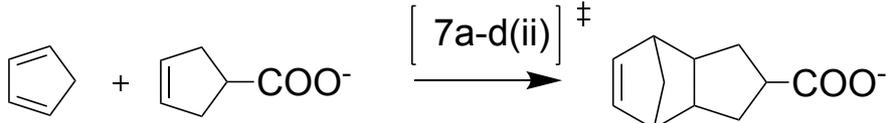
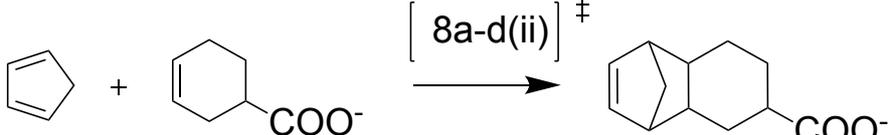
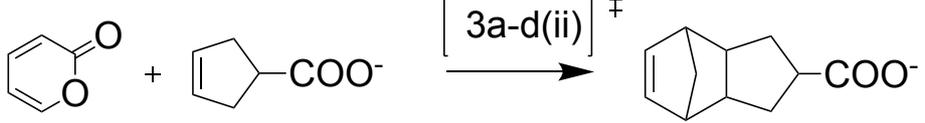
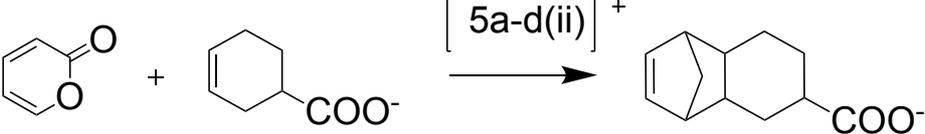
									
T=298.15K	ΔE^\ddagger_{M06}	ΔH^\ddagger_{M06}	ΔH_{M06}	ΔG^\ddagger_{M06}	ΔG^\ddagger_{G3}	ΔG_{M06}	ΔS^\ddagger_{M06}	ΔS_{M06}	iFreq _{M06}
a	69.6	74.2	-101.9	132.9	121.2	-38.4	-197.0	-209.3	-492.2
b	60.8	64.8	-102.7	129.7	116.3	-38.3	-217.7	-212.9	-527.3
c	73.4	77.6	-105.3	135.5	126.9	-42.5	-194.3	-207.7	-499.9
d	68.6	72.7	-113.3	132.7	122.8	-48.5	-201.1	-212.9	-517.6
									
T=298.15K	ΔE^\ddagger_{M06}	ΔH^\ddagger_{M06}	ΔH_{M06}	ΔG^\ddagger_{M06}	ΔG^\ddagger_{G3}	ΔG_{M06}	ΔS^\ddagger_{M06}	ΔS_{M06}	iFreq _{M06}
a	86.1	74.2	-101.9	132.9	137.2	-5.6	-179.4	-194.7	-502.2
b	92.9	64.8	-102.7	129.7	143.1	-25.2	-172.9	-195.1	-456.2
c	88.6	77.6	-105.3	135.5	140.8	-10.4	-182.7	-195.2	-498.9
d	77.9	72.7	-113.3	132.7	134.2	-28.6	-197.0	-194.4	-531.7
									
T=298.15K	ΔE^\ddagger_{M06}	ΔH^\ddagger_{M06}	ΔH_{M06}	ΔG^\ddagger_{M06}	ΔG^\ddagger_{G3}	ΔG_{M06}	ΔS^\ddagger_{M06}	ΔS_{M06}	iFreq _{M06}
a	38.9	74.2	-142.6	132.9	94.2	-77.3	-164.6	-181.2	-500.6
b	17.4	64.8	-145.9	129.7	99.6	-79.8	-188.8	-182.8	-544.8
c	60.7	77.6	-129.7	135.5	115.9	-63.7	-164.2	-183.1	-488.6
d	83.0	72.7	-130.0	132.7	136.3	-65.3	-168.0	-184.2	-502.6
									
T=298.15K	ΔE^\ddagger_{M06}	ΔH^\ddagger_{M06}	ΔH_{M06}	ΔG^\ddagger_{M06}	ΔG^\ddagger_{G3}	ΔG_{M06}	ΔS^\ddagger_{M06}	ΔS_{M06}	iFreq _{M06}
a	56.2	56.2	-112.2	118.1	110.0	-46.1	-146.9	-167.8	-476.7
b	38.3	38.3	-123.6	120.0	99.6	-59.1	-169.2	-165.8	-567.1
c	56.8	56.8	-113.5	108.8	112.8	-47.3	-148.8	-168.6	-536.5
d	33.3	33.3	-124.4	103.6	94.4	-60.2	-168.9	-165.5	-558.7
e	65.0	65.0	-96.2	129.4	121.2	-30.2	-152.2	-169.7	-477.0
f	79.0	79.0	-114.4	130.0	135.4	-50.2	-153.3	-165.6	-511.2
g	66.5	66.5	-94.0	147.0	121.1	-28.0	-150.6	-170.0	-479.1
h	86.8	86.8	-112.6	143.3	139.6	-48.5	-141.9	-166.1	-451.0

Table S3: Kinetic and thermodynamic parameters (kJ mol⁻¹) and the imaginary frequency for each transition state, calculated at M062X/6-31+G** (M06) and G3(MP2)-CC (G3) where R=NMe₂

T=298.15K	ΔE^\ddagger_{M06}	ΔH^\ddagger_{M06}	ΔH_{M06}	ΔG^\ddagger_{M06}	ΔG^\ddagger_{G3}	ΔG_{M06}	ΔS^\ddagger_{M06}	ΔS_{M06}	iFreq_{M06}
a	61.0	64.7	-112.0	125.8	115.4	-46.5	-195.2	-198.2	-505.0
b	71.0	74.7	-112.2	134.0	124.7	-47.3	-189.0	-199.0	-509.0
c	74.3	78.5	-110.3	138.1	128.2	-46.0	-190.3	-196.5	-504.5
d	82.8	87.3	-108.6	147.1	139.3	-43.8	-190.7	-200.4	-517.4
T=298.15K	ΔE^\ddagger_{M06}	ΔH^\ddagger_{M06}	ΔH_{M06}	ΔG^\ddagger_{M06}	ΔG^\ddagger_{G3}	ΔG_{M06}	ΔS^\ddagger_{M06}	ΔS_{M06}	iFreq_{M06}
a	88.0	64.7	-71.6	149.8	139.7	-7.5	-165.4	-179.4	-537.1
b	92.0	74.7	-89.6	154.5	144.1	-27.3	-168.5	-179.9	-473.9
c	95.5	78.5	-70.7	157.9	147.9	-5.3	-167.0	-182.3	-531.3
d	100.0	87.3	-89.5	162.8	152.4	-27.6	-169.4	-179.4	-477.3
T=298.15K	ΔE^\ddagger_{M06}	ΔH^\ddagger_{M06}	ΔH_{M06}	ΔG^\ddagger_{M06}	ΔG^\ddagger_{G3}	ΔG_{M06}	ΔS^\ddagger_{M06}	ΔS_{M06}	iFreq_{M06}
a	64.4	66.8	-121.4	129.4	120.5	-54.8	-163.8	-169.5	-530.6
b	73.4	75.8	-124.0	136.9	148.2	-57.6	-158.8	-169.1	-537.8
c	61.7	64.6	-127.4	128.6	119.7	-60.1	-168.4	-171.2	-524.4
d	77.9	80.9	-125.1	143.1	136.8	-58.8	-162.6	-169.9	-538.5
T=298.15K	ΔE^\ddagger_{M06}	ΔH^\ddagger_{M06}	ΔH_{M06}	ΔG^\ddagger_{M06}	ΔG^\ddagger_{G3}	ΔG_{M06}	ΔS^\ddagger_{M06}	ΔS_{M06}	iFreq_{M06}
a	92.4	96.8	-84.7	154.9	147.5	-18.8	-136.3	-152.6	-560.6
b	94.0	95.6	-97.7	152.1	148.2	-33.7	-137.2	-150.9	-508.1
c	89.9	92.8	-84.6	156.4	144.8	-18.4	-136.2	-153.2	-560.4
d	93.5	96.7	-97.8	156.6	147.4	-34.3	-138.2	-150.6	-504.8
e	87.9	91.4	-87.3	153.6	144.5	-22.3	-145.8	-153.4	-561.0
f	94.0	97.1	-99.2	152.9	149.9	-34.8	-139.2	-150.8	-497.4
g	87.6	91.8	-86.7	154.5	144.3	-21.3	-142.1	-153.3	-549.8
h	94.4	97.3	-99.0	157.2	149.2	-36.7	-129.5	-150.9	-506.2

Table S4: Kinetic and thermodynamic parameters (kJ mol⁻¹) and the imaginary frequency for each transition state, calculated at M062X/6-31+G** (M06) and G3(MP2)-CC (G3) where R=NMe₂H⁺

T=298.15K	ΔE^\ddagger_{M06}	ΔH^\ddagger_{M06}	ΔH_{M06}	ΔG^\ddagger_{M06}	ΔG^\ddagger_{G3}	ΔG_{M06}	ΔS^\ddagger_{M06}	ΔS_{M06}	iFreq_{M06}
a	50.7	54.2	-122.5	111.6	103.5	-60.6	-190.4	-194.3	-501.7
b	58.3	62.2	-120.7	118.1	112.0	-59.4	-185.2	-195.8	-495.8
c	71.1	75.2	-112.9	133.0	126.0	-52.2	-191.5	-192.5	-509.2
d	71.0	75.0	-114.1	132.0	125.6	-51.6	-189.0	-198.5	-501.2
T=298.15K	ΔE^\ddagger_{M06}	ΔH^\ddagger_{M06}	ΔH_{M06}	ΔG^\ddagger_{M06}	ΔG^\ddagger_{G3}	ΔG_{M06}	ΔS^\ddagger_{M06}	ΔS_{M06}	iFreq_{M06}
a	79.5	83.1	-80.4	140.3	130.4	-17.2	-168.8	-178.8	-534.6
b	83.8	87.3	-94.2	143.5	135.7	-33.5	-165.3	-177.8	-470.4
c	94.8	98.7	-72.6	155.7	146.0	-9.3	-168.1	-179.2	-524.5
d	92.3	96.3	-90.4	152.8	143.6	-30.6	-166.6	-177.3	-524.8
T=298.15K	ΔE^\ddagger_{M06}	ΔH^\ddagger_{M06}	ΔH_{M06}	ΔG^\ddagger_{M06}	ΔG^\ddagger_{G3}	ΔG_{M06}	ΔS^\ddagger_{M06}	ΔS_{M06}	iFreq_{M06}
a	92.2	94.3	-95.7	153.2	143.9	-32.7	-159.1	-165.2	-553.2
b	99.3	101.3	-95.9	158.9	169.4	-33.2	-154.9	-165.5	-549.8
c	52.6	55.9	-125.2	118.1	110.3	-60.7	-170.1	-169.1	-555.7
d	18.6	19.9	-117.6	84.3	76.9	-55.7	-177.5	-169.4	-551.2
T=298.15K	ΔE^\ddagger_{M06}	ΔH^\ddagger_{M06}	ΔH_{M06}	ΔG^\ddagger_{M06}	ΔG^\ddagger_{G3}	ΔG_{M06}	ΔS^\ddagger_{M06}	ΔS_{M06}	iFreq_{M06}
a	120.4	120.4	-60.0	180.4	170.8	4.8	-134.5	-151.4	-578.2
b	118.3	122.6	-71.1	170.5	169.4	-9.3	-136.2	-148.3	-530.3
c	108.6	111.3	-58.9	178.8	161.0	6.0	-139.3	-152.0	-578.1
d	118.6	120.6	-70.2	179.1	169.5	-8.4	-136.6	-148.2	-526.8
e	78.3	81.8	-90.3	143.8	134.3	-24.6	-148.6	-154.0	-586.8
f	38.0	39.3	-87.7	134.0	94.9	-23.0	-158.7	-153.5	-565.4
g	66.3	70.7	-89.6	107.1	127.4	-24.4	-153.1	-154.0	-575.4
h	39.9	41.7	-87.2	104.4	98.2	-23.5	-159.9	-152.5	-552.6

Table S5: Kinetic and thermodynamic pH-switches (kJ mol⁻¹) between neutral (R=COOH) and deprotonated (R=COO⁻) species calculated at M062X/6-31+G^{**}. A negative $\Delta\Delta G^\ddagger$ corresponds to a lower activation barrier when charged.

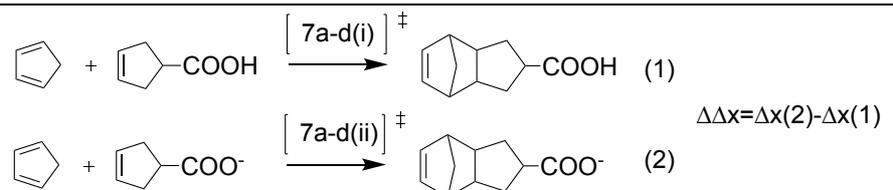
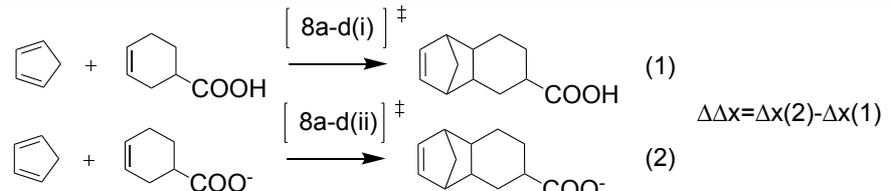
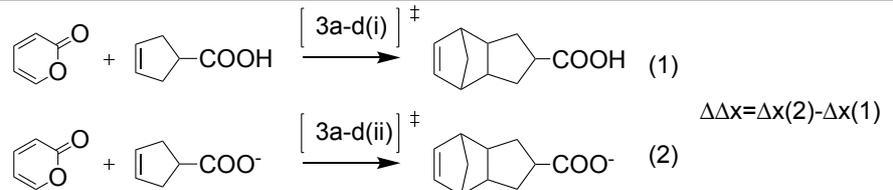
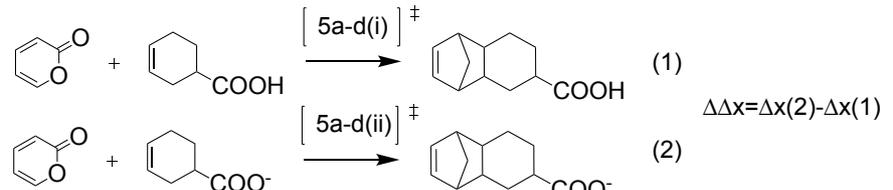
								
	$\Delta\Delta E^\ddagger$	$\Delta\Delta E$	$\Delta\Delta H^\ddagger$	$\Delta\Delta H$	$\Delta\Delta G^\ddagger$	$\Delta\Delta G$	$\Delta\Delta S^\ddagger$	$\Delta\Delta S$
a	2.3	-0.1	2.7	4.1	2.6	4.7	0.8	-3.3
b	-10.0	-12.3	-10.0	2.4	-7.7	3.4	-7.4	-2.9
c	-7.5	-8.0	-7.7	-3.2	-7.4	-2.3	-0.7	-3.1
d	-12.6	-15.8	-13.4	-3.9	-12.6	-1.7	-2.1	-3.9
								
	$\Delta\Delta E^\ddagger$	$\Delta\Delta E$	$\Delta\Delta H^\ddagger$	$\Delta\Delta H$	$\Delta\Delta G^\ddagger$	$\Delta\Delta G$	$\Delta\Delta S^\ddagger$	$\Delta\Delta S$
a	1.1	-0.8	1.3	3.9	1.3	3.9	-2.1	-3.1
b	2.3	-0.4	2.4	2.3	1.8	2.5	-0.3	-3.2
c	-6.0	-7.5	-5.8	-2.5	-4.4	-2.2	-6.9	-3.2
d	-15.5	-13.1	-15.0	-1.2	-8.9	-0.7	-22.2	-3.3
								
	$\Delta\Delta E^\ddagger$	$\Delta\Delta E$	$\Delta\Delta H^\ddagger$	$\Delta\Delta H$	$\Delta\Delta G^\ddagger$	$\Delta\Delta G$	$\Delta\Delta S^\ddagger$	$\Delta\Delta S$
a	-34.8	-35.2	-34.6	-30.1	-35.4	-29.1	3.2	-3.0
b	-56.5	-49.7	-56.0	-31.3	-53.4	-29.5	-8.3	-3.8
c	-7.6	-10.6	-8.2	-10.7	-11.2	-10.3	10.2	-2.5
d	4.0	-4.6	3.4	-14.8	-2.0	-15.5	18.9	-2.0
								
	$\Delta\Delta E^\ddagger$	$\Delta\Delta E$	$\Delta\Delta H^\ddagger$	$\Delta\Delta H$	$\Delta\Delta G^\ddagger$	$\Delta\Delta G$	$\Delta\Delta S^\ddagger$	$\Delta\Delta S$
a	-35.3	-35.2	-8.2	-27.9	-38.1	-27.5	5.3	-3.4
b	-56.3	-49.7	3.4	-27.4	-33.3	-26.6	-25.1	-3.6
c	-34.0	-10.6	-8.2	-29.2	-47.9	-28.7	-3.2	-3.3
d	-59.1	-4.6	3.4	-28.7	-51.2	-28.0	-24.6	-3.7
e	-18.9	-35.2	-8.2	-8.6	-21.7	-7.5	7.4	-2.6
f	-8.2	-49.7	3.4	-17.9	-22.1	-17.1	3.0	-2.9
g	-18.7	-10.6	-8.2	-7.1	-10.3	-6.7	8.7	-2.5
h	-4.8	-4.6	3.4	-16.3	-10.1	-14.9	13.7	-2.5

Table S6: Kinetic and thermodynamic pH-switches (kJ mol⁻¹) between neutral (R=NMe₂) and protonated (R=NMe₂H⁺) species calculated at M062X/6-31+G^{**}. A negative $\Delta\Delta G^\ddagger$ corresponds to a lower activation barrier when charged.

<p style="text-align: right;">$\Delta\Delta x = \Delta x(2) - \Delta x(1)$</p>								
	$\Delta\Delta E^\ddagger$	$\Delta\Delta E$	$\Delta\Delta H^\ddagger$	$\Delta\Delta H$	$\Delta\Delta G^\ddagger$	$\Delta\Delta G$	$\Delta\Delta S^\ddagger$	$\Delta\Delta S$
a	-10.3	-11.9	-10.5	-10.6	-14.2	-14.1	4.8	3.8
b	-12.7	-12.7	-12.5	-8.5	-16.0	-12.1	3.8	3.2
c	-3.1	-2.2	-3.2	-2.7	-5.1	-6.2	-1.2	3.9
d	-11.8	-13.7	-12.4	-5.5	-15.1	-7.8	1.7	1.9
<p style="text-align: right;">$\Delta\Delta x = \Delta x(2) - \Delta x(1)$</p>								
	$\Delta\Delta E^\ddagger$	$\Delta\Delta E$	$\Delta\Delta H^\ddagger$	$\Delta\Delta H$	$\Delta\Delta G^\ddagger$	$\Delta\Delta G$	$\Delta\Delta S^\ddagger$	$\Delta\Delta S$
a	-8.6	-9.3	-9.5	-8.9	-9.4	-9.7	-3.4	0.6
b	-8.2	-8.4	-9.0	-4.6	-10.9	-6.2	3.2	2.0
c	-0.7	-2.0	-1.6	-1.8	-2.2	-4.0	-1.1	3.1
d	-7.7	-8.8	-8.2	-0.9	-10.0	-2.9	2.8	2.1
<p style="text-align: right;">$\Delta\Delta x = \Delta x(2) - \Delta x(1)$</p>								
	$\Delta\Delta E^\ddagger$	$\Delta\Delta E$	$\Delta\Delta H^\ddagger$	$\Delta\Delta H$	$\Delta\Delta G^\ddagger$	$\Delta\Delta G$	$\Delta\Delta S^\ddagger$	$\Delta\Delta S$
a	27.9	23.5	27.5	25.7	23.8	22.1	4.6	4.3
b	25.9	21.2	25.5	28.1	22.0	24.4	4.0	3.6
c	-9.1	-9.4	-8.8	2.2	-10.5	-0.6	-1.7	2.1
d	-59.2	-60.0	-61.0	7.5	-58.8	3.1	-14.9	0.5
<p style="text-align: right;">$\Delta\Delta x = \Delta x(2) - \Delta x(1)$</p>								
	$\Delta\Delta E^\ddagger$	$\Delta\Delta E$	$\Delta\Delta H^\ddagger$	$\Delta\Delta H$	$\Delta\Delta G^\ddagger$	$\Delta\Delta G$	$\Delta\Delta S^\ddagger$	$\Delta\Delta S$
a	28.0	23.2	23.6	24.7	25.5	23.5	1.8	1.1
b	24.3	21.2	27.0	26.5	18.4	24.4	1.0	2.6
c	18.7	16.2	18.4	25.8	22.4	24.4	-3.1	1.2
d	25.0	22.1	23.9	27.6	22.5	25.9	1.5	2.4
e	-9.6	-10.2	-9.7	-3.1	-9.8	-2.3	-2.8	-0.5
f	-56.0	-55.0	-57.7	11.5	-18.8	11.8	-19.5	-2.8
g	-21.3	-16.9	-21.1	-2.9	-47.4	-3.2	-11.0	-0.7
h	-54.5	-51.0	-55.6	11.8	-52.9	13.2	-30.4	-1.6

Table S7: Distortion/Interaction analysis (kJ mol^{-1}), transition state bond lengths (\AA) and the Mulliken charge of the diene transition state fragment where $\text{R}=\text{COOH}$

	r1(\AA)	r2(\AA)	Distortion ΔE	Interaction ΔE	Diene Distortion ΔE	Dienophile Distortion ΔE	Charge diene
a	2.21	2.22	108.8	-41.5	69.2	39.7	0.144
b	2.22	2.20	116.7	-45.9	69.5	47.2	0.134
c	2.23	2.23	117.0	-36.0	71.5	45.5	0.092
d	2.22	2.10	123.5	-42.3	72.1	51.3	0.080
	r1(\AA)	r2(\AA)	Distortion ΔE	Interaction ΔE	Diene Distortion ΔE	Dienophile Distortion ΔE	Charge diene
a	2.16	2.24	126.7	-41.7	75.0	51.7	0.105
b	2.25	2.22	129.3	-38.7	65.4	63.9	0.210
c	2.21	2.21	130.9	-36.3	75.8	55.0	0.099
d	2.21	2.20	130.6	-37.1	75.7	54.9	0.108
	r1(\AA)	r2(\AA)	Distortion ΔE	Interaction ΔE	Diene Distortion ΔE	Dienophile Distortion ΔE	Charge diene
a	2.30	2.13	127.3	-53.6	85.3	42.0	-0.10
b	2.28	2.13	135.7	-61.7	85.7	50.0	-0.10
c	2.11	2.36	127.4	-60.5	85.3	43.5	-0.07
d	2.10	2.34	135.7	-63.8	88.2	54.7	-0.09
	r1(\AA)	r2(\AA)	Distortion ΔE	Interaction ΔE	Diene Distortion ΔE	Dienophile Distortion ΔE	Charge diene
a	2.33	2.07	127.3	-56.7	92.2	56.1	-0.10
b	2.33	2.12	135.7	-55.1	82.6	67.0	-0.04
c	2.08	2.32	127.4	-56.9	92.5	55.2	-0.14
d	2.12	2.26	135.7	-57.6	94.2	55.8	-0.14
e	2.10	2.32	128.8	-64.5	92.1	56.3	-0.11
f	2.10	2.30	142.8	-63.3	94.0	56.4	-0.12
g	2.34	2.09	127.3	-66.3	95.4	56.1	-0.13
h	2.32	2.09	135.7	-62.0	96.5	57.0	-0.14

Table S8: Distortion/Interaction analysis (kJ mol^{-1}), transition state bond lengths (\AA) and the mulliken charge of the diene transition state fragment where $\text{R}=\text{COO}^-$

	r1(\AA)	r2(\AA)	Distortion ΔE	Interaction ΔE	Diene Distortion ΔE	Dienophile Distortion ΔE	Charge diene
a	2.23	2.23	104.2	-34.5	69.0	35.2	0.019
b	2.21	2.21	115.5	-54.7	72.3	43.2	0.033
c	2.23	2.23	110.8	-37.4	71.5	39.3	-0.060
d	2.22	2.22	119.6	-51.0	73.4	46.1	-0.010
	r1(\AA)	r2(\AA)	Distortion ΔE	Interaction ΔE	Diene Distortion ΔE	Dienophile Distortion ΔE	Charge diene
a	2.26	2.18	119.6	-33.5	73.4	46.2	0.003
b	2.25	2.23	124.4	-31.5	65.5	58.9	0.081
c	2.22	2.23	123.0	-34.4	74.4	48.6	0.004
d	2.19	2.23	139.0	-61.1	79.9	59.0	0.051
	r1(\AA)	r2(\AA)	Distortion ΔE	Interaction ΔE	Diene Distortion ΔE	Dienophile Distortion ΔE	Charge diene
a	2.39	2.10	120.7	-81.8	85.5	35.1	-0.24
b	2.32	2.10	135.8	-118.4	90.8	45.0	-0.22
c	2.09	2.46	121.4	-60.7	84.6	36.8	-0.23
d	2.09	2.48	138.0	-55.0	84.0	54.1	-0.23
	r1(\AA)	r2(\AA)	Distortion ΔE	Interaction ΔE	Diene Distortion ΔE	Dienophile Distortion ΔE	Charge diene
a	2.61	2.00	144.6	-88.3	92.2	52.4	-0.33
b	2.30	2.08	158.1	-119.8	98.9	59.1	-0.19
c	2.04	2.41	144.8	-88.0	94.4	50.5	-0.25
d	2.05	2.36	157.5	-124.2	97.8	59.7	-0.19
e	2.09	2.44	139.0	-74.0	89.7	49.3	-0.26
f	2.09	2.36	144.6	-65.6	93.6	51.0	-0.24
g	2.56	2.06	142.0	-75.5	90.3	51.7	-0.29
h	2.47	2.12	142.3	-55.5	79.6	62.7	-0.13

Table S9: Distortion/Interaction analysis (kJ mol^{-1}), transition state bond lengths (\AA) and the Mulliken charge of the diene transition state fragment where $\text{R}=\text{NMe}_2$

	r1(\AA)	r2(\AA)	Distortion ΔE	Interaction ΔE	Diene Distortion ΔE	Dienophile Distortion ΔE	Charge diene
a	2.22	2.22	101.4	-40.4	69.2	32.2	0.106
b	2.22	2.22	109.9	-38.9	66.9	43.0	0.099
c	2.24	2.24	108.9	-34.7	71.0	37.9	0.070
d	2.22	2.23	119.5	-36.7	70.0	49.5	0.060
	r1(\AA)	r2(\AA)	Distortion ΔE	Interaction ΔE	Diene Distortion ΔE	Dienophile Distortion ΔE	Charge diene
a	2.16	2.23	128.8	-40.7	75.5	53.2	0.115
b	2.22	2.24	129.8	-37.7	66.0	63.8	0.209
c	2.22	2.21	131.8	-36.3	76.0	55.8	0.095
d	2.25	2.24	133.6	-33.7	68.0	65.6	0.171
	r1(\AA)	r2(\AA)	Distortion ΔE	Interaction ΔE	Diene Distortion ΔE	Dienophile Distortion ΔE	Charge diene
a	2.30	2.13	119.9	-55.5	85.5	34.4	-0.13
b	2.31	2.13	129.7	-56.4	83.7	46.1	-0.15
c	2.12	2.36	120.9	-55.5	85.4	35.5	-0.11
d	2.12	2.36	141.2	-56.4	87.3	53.9	-0.13
	r1(\AA)	r2(\AA)	Distortion ΔE	Interaction ΔE	Diene Distortion ΔE	Dienophile Distortion ΔE	Charge diene
a	2.27	2.11	150.7	-58.3	94.9	55.9	-0.14
b	2.34	2.11	149.9	-55.9	82.9	66.9	-0.04
c	2.07	2.32	148.5	-58.6	93.0	55.5	-0.15
d	2.13	2.33	149.1	-55.5	82.7	66.4	-0.04
e	2.08	2.33	154.0	-66.1	97.5	56.5	-0.14
f	2.14	2.34	153.8	-59.8	84.6	69.2	-0.02
g	2.32	2.09	152.0	-64.4	94.9	57.1	-0.11
h	2.40	2.10	153.1	-58.7	84.5	68.6	-0.02

Table S10: Distortion/Interaction analysis (kJ mol^{-1}), transition state bond lengths (\AA) and the mulliken charge of the diene transition state fragment where $\text{R}=\text{NMe}_2\text{H}^+$

	r1(\AA)	r2(\AA)	Distortion ΔE	Interaction ΔE	Diene Distortion ΔE	Dienophile Distortion ΔE	Charge diene
a	2.22	2.22	114.1	-63.5	68.7	45.5	0.240
b	2.22	2.22	120.9	-62.6	65.0	56.0	0.240
c	2.22	2.22	126.7	-55.6	70.3	56.5	0.283
d	2.23	2.23	123.3	-52.3	67.8	55.4	0.214
	r1(\AA)	r2(\AA)	Distortion ΔE	Interaction ΔE	Diene Distortion ΔE	Dienophile Distortion ΔE	Charge diene
a	2.16	2.23	139.8	-60.3	75.3	64.4	0.240
b	2.24	2.22	142.1	-58.3	65.2	76.9	0.348
c	2.21	2.20	144.8	-50.0	75.5	69.3	0.217
d	2.23	2.19	143.1	-50.8	75.3	67.9	0.588
	r1(\AA)	r2(\AA)	Distortion ΔE	Interaction ΔE	Diene Distortion ΔE	Dienophile Distortion ΔE	Charge diene
a	2.24	2.16	136.5	-44.3	85.3	51.2	0.01
b	2.24	2.16	145.2	-45.9	81.1	64.1	0.03
c	2.10	2.32	142.4	-89.8	88.7	53.7	0.03
d	2.03	2.45	165.5	-146.8	95.1	70.3	0.03
	r1(\AA)	r2(\AA)	Distortion ΔE	Interaction ΔE	Diene Distortion ΔE	Dienophile Distortion ΔE	Charge diene
a	2.23	2.14	166.0	-45.6	94.1	72.0	0.00
b	2.25	2.15	166.7	-48.4	82.5	84.2	0.11
c	2.16	2.17	158.9	-50.4	91.4	67.5	0.10
d	2.16	2.25	164.9	-46.3	81.5	83.3	0.12
e	2.08	2.31	174.7	-96.4	101.1	73.5	-0.01
f	2.02	2.42	187.2	-149.2	105.0	82.2	0.03
g	2.30	2.07	175.1	-108.8	100.7	74.4	-0.02
h	2.38	2.04	190.1	-150.2	102.8	87.3	0.05

Table S11: Solvent dependence of the pH-switch ($\Delta\Delta G^\ddagger$) calculated for each conformer reaction of 2-pyrone with neutral and deprotonated 3-cyclopentenecarboxylic acid and the reaction of 2-pyrone with neutral and protonated N,N-dimethylcyclopent-3-en-1-amine. A negative $\Delta\Delta G^\ddagger$ corresponds to a lower activation barrier when charged.

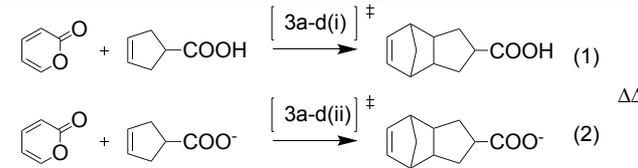
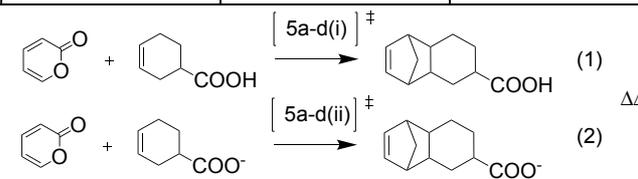
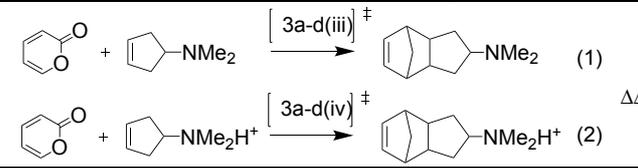
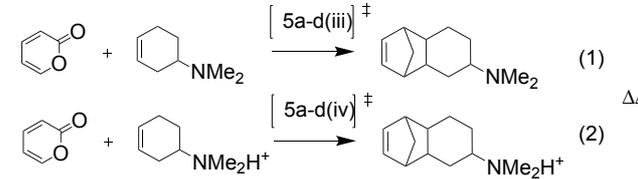
						
	$\Delta\Delta G^\ddagger_{\text{TOL}}$	$\Delta\Delta G^\ddagger_{\text{THF}}$	$\Delta\Delta G^\ddagger_{\text{DCM}}$	$\Delta\Delta G^\ddagger_{\text{PY}}$	$\Delta\Delta G^\ddagger_{\text{ACN}}$	$\Delta\Delta G^\ddagger_{\text{H}_2\text{O}}$
a	-18.0	-8.3	-6.9	-5.5	-3.8	-1.4
b	-24.6	-8.7	-5.7	-5.3	-1.2	1.5
c	-3.9	-3.6	-3.0	-4.2	-4.8	-4.4
d	1.8	-0.1	1.2	-1.5	-1.7	4.4
						
	$\Delta\Delta G^\ddagger_{\text{TOL}}$	$\Delta\Delta G^\ddagger_{\text{THF}}$	$\Delta\Delta G^\ddagger_{\text{DCM}}$	$\Delta\Delta G^\ddagger_{\text{PY}}$	$\Delta\Delta G^\ddagger_{\text{ACN}}$	$\Delta\Delta G^\ddagger_{\text{H}_2\text{O}}$
a	-19.8	-10.1	-9.8	-8.3	-6.9	-8.2
b	-15.9	2.4	3.8	6.2	9.7	7.7
c	-16.4	-5.8	-5.4	-3.5	-1.5	-2.1
d	-20.0	-1.5	-0.3	2.4	5.8	5.5
e	-9.6	-3.4	-3.5	-2.4	-1.7	-3.5
f	-3.5	-1.6	-2.1	-2.0	-2.5	-2.8
g	-10.1	-4.5	-4.8	-3.7	-3.1	-4.7
h	-3.3	-1.0	-1.1	-1.2	-1.1	-0.9
						
	$\Delta\Delta G^\ddagger_{\text{TOL}}$	$\Delta\Delta G^\ddagger_{\text{THF}}$	$\Delta\Delta G^\ddagger_{\text{DCM}}$	$\Delta\Delta G^\ddagger_{\text{PY}}$	$\Delta\Delta G^\ddagger_{\text{ACN}}$	$\Delta\Delta G^\ddagger_{\text{H}_2\text{O}}$
a	18.4	9.5	8.5	6.9	4.4	3.7
b	18.7	10.6	9.5	7.9	5.2	4.5
c	1.3	4.3	4.2	4.6	4.7	5.6
d	-31.7	-14.3	-13.1	-10.5	-6.8	-2.9
						
	$\Delta\Delta G^\ddagger_{\text{TOL}}$	$\Delta\Delta G^\ddagger_{\text{THF}}$	$\Delta\Delta G^\ddagger_{\text{DCM}}$	$\Delta\Delta G^\ddagger_{\text{PY}}$	$\Delta\Delta G^\ddagger_{\text{ACN}}$	$\Delta\Delta G^\ddagger_{\text{H}_2\text{O}}$
a	15.4	4.5	3.3	1.5	-1.3	-1.5
b	14.5	5.3	4.4	2.7	0.5	1.4
c	13.9	7.2	6.7	5.4	3.9	4.4
d	14.2	4.0	3.0	1.1	-1.7	-1.0
e	-2.4	-0.8	-1.1	-0.8	-0.9	0.1
f	-27.7	-12.6	-11.8	-9.4	-6.7	-4.6
g	-5.9	-1.5	-1.3	-0.8	-0.3	2.2
h	-21.7	-6.6	-6.2	-3.4	-0.9	-0.2

Figure S1: pi-pi* energies (eV) for both Normal and Inverse Electron demand reactivity calculated for each of the distorted transition state diene (2-pyrone) and dienophile (3-substituted cyclopentene) fragments at M062X/6-31+G**

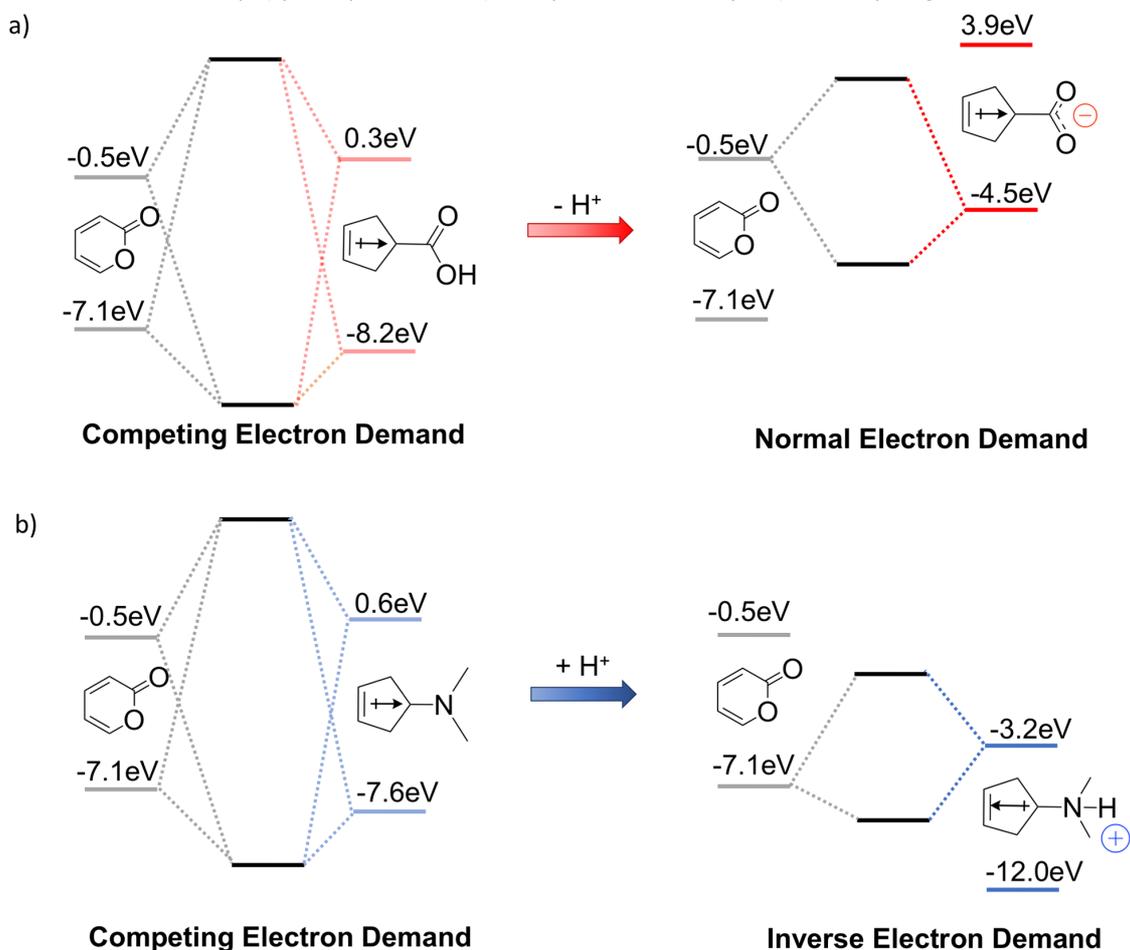


Table S12: pi-pi* energies (eV) for both Normal and Inverse Electron demand reactivity calculated for each of the distorted transition state diene (2-pyrone) and dienophile (3-substituted cyclopentene) fragments where R is the charged functional group substituted at the 3 position of cyclopentene at M062X/6-31+G**

	$\Delta E(\pi^*(\text{dienophile})-\pi(\text{diene}))$ [eV]				$\Delta E(\pi^*(\text{dine})-\pi(\text{dienophile}))$ [eV]			
	R=COOH	R=COO ⁻	R=NMe ₂	R=NMe ₂ H ⁺	R=COOH	R=COO ⁻	R=NMe ₂	R=NMe ₂ H ⁺
a	6.4	2.7	5.9	10.2	8.2	11.7	8.5	4.6
b	6.3	2.5	6.1	10.2	8.4	11.8	8.4	4.4
c	6.4	2.6	5.9	10.1	8.2	11.6	8.5	4.6
d	6.3	2.7	6.1	10.0	8.4	11.5	8.4	4.7

Table S13: Components of the G3(MP2)-CC calculation(in hartrees unless stated otherwise) for every starting material calculated

	Entropy(J/mol K)	TC	ZPVE	HLC	SO	M062X/6-31+G**	MP2/6-31G*	MP2/large	URCCSD(T)/6-31G*	E	H	G
6	273.2921	0.0051	0.0934	-0.1224	0.0000	-194.0195	-193.4252	-193.6479	-193.4944	-193.8394	-193.7409	-193.7719
1	309.6706	0.0062	0.0814	-0.1694	0.0000	-343.2405	-342.3517	-342.7163	-342.4218	-342.9559	-342.8683	-342.9035
2(ii)	347.2325	0.0079	0.1194	-0.2071	0.0000	-383.1981	-382.1388	-382.5919	-382.2279	-382.8882	-382.7610	-382.8004
2(i)	350.4862	0.0081	0.1335	-0.2071	0.0000	-383.7574	-382.7108	-383.1497	-382.8035	-383.4495	-383.3079	-383.3477
2(iii)	365.9572	0.0092	0.1918	-0.2165	0.0000	-329.1451	-328.1202	-328.5283	-328.2387	-328.8633	-328.6623	-328.7039
2(iv)	363.5527	0.0091	0.2074	-0.2165	0.0000	-329.5270	-328.5073	-328.9105	-328.6281	-329.2478	-329.0313	-329.0726
4(ii)	365.3443	0.0088	0.1487	-0.2353	0.0000	-422.5036	-421.3138	-421.8190	-421.4191	-422.1595	-422.0020	-422.0435
4(i)	369.2394	0.0091	0.1630	-0.2353	0.0000	-423.0619	-421.8843	-422.3757	-421.9931	-422.7198	-422.5478	-422.5897
4(iii)	384.1685	0.0101	0.2213	-0.2447	0.0000	-368.4497	-367.2942	-367.7543	-367.4287	-368.1335	-367.9021	-367.9457
4(iv)	381.6281	0.0100	0.2374	-0.2447	0.0000	-368.8339	-367.6840	-368.1395	-367.8204	-368.5207	-368.2733	-368.3166

Table S14: Components of the G3(MP2)-CC calculation in hartrees unless stated otherwise for every product calculated

	Entropy(J/mol K)	TC	ZPVE	HLC	SO	M062X/6-31+G**	MP2/6-31G*	MP2/large	URCCSD(T)/6-31G*	E	H	G
7a(ii)[product]	407.9159	0.0108	0.2208	-0.3295	0.0000	-577.2623	-575.6203	-576.2951	-575.7687	-576.7730	-576.5414	-576.5877
7a(i) [product]	411.2369	0.0110	0.2349	-0.3295	0.0000	-577.8232	-576.1933	-576.8534	-576.3456	-577.3351	-577.0892	-577.1359
7a(iii) [product]	422.3722	0.0120	0.2933	-0.3389	0.0000	-523.2131	-521.6055	-522.2343	-521.7835	-522.7511	-522.4459	-522.4938
7a(iv) [product]	426.2174	0.0122	0.3088	-0.3389	0.0000	-523.5992	-521.9966	-522.6204	-522.1773	-523.1399	-522.8189	-522.8673
8a(ii) [product]	422.6953	0.0117	0.2505	-0.3577	0.0000	-616.5558	-614.7831	-615.5103	-614.9476	-616.0326	-615.7704	-615.8184
8a(i) [product]	425.7937	0.0119	0.2649	-0.3577	0.0000	-617.1157	-615.3550	-616.0679	-615.5232	-616.5938	-616.3170	-616.3654
8a(iii) [product]	441.1208	0.0130	0.3228	-0.3671	0.0000	-562.5024	-560.7635	-561.4454	-560.9575	-562.0065	-561.6707	-561.7207
8a(iv) [product]	441.7475	0.0130	0.3387	-0.3671	0.0000	-562.8899	-561.1563	-561.8334	-561.3529	-562.3971	-562.0454	-562.0955
7b(ii) [product]	404.7602	0.0107	0.2209	-0.3295	0.0000	-577.2627	-575.6207	-576.2956	-575.7692	-576.7735	-576.5419	-576.5879
7b(i) [product]	407.6481	0.0109	0.2351	-0.3295	0.0000	-577.8229	-576.1931	-576.8533	-576.3455	-577.3352	-577.0892	-577.1355
7b(iii) [product]	421.5343	0.0119	0.2933	-0.3389	0.0000	-523.2132	-521.6055	-522.2346	-521.7836	-522.7516	-522.4463	-522.4942
7b(iv) [product]	424.7608	0.0121	0.3090	-0.3389	0.0000	-523.5986	-521.9957	-522.6197	-522.1765	-523.1394	-522.8184	-522.8666
8b(ii) [product]	422.2231	0.0117	0.2503	-0.3577	0.0000	-616.5625	-614.7898	-615.5169	-614.9544	-616.0392	-615.7773	-615.8253
8b(i) [product]	425.4398	0.0119	0.2646	-0.3577	0.0000	-617.1217	-615.3610	-616.0740	-615.5294	-616.6001	-616.3235	-616.3718
8b(iii) [product]	440.6627	0.0130	0.3227	-0.3671	0.0000	-562.5091	-560.7702	-561.4523	-560.9644	-562.0135	-561.6779	-561.7279
8b(iv) [product]	442.6769	0.0131	0.3385	-0.3671	0.0000	-562.8950	-561.1613	-561.8386	-561.3581	-562.4025	-562.0509	-562.1011

7c(ii)[product]	409.7413	0.0109	0.2209	-0.3295	0.0000	-577.2637	-575.6218	-576.2964	-575.7706	-576.7747	-576.5430	-576.5895
7c(i) [product]	412.8734	0.0111	0.2350	-0.3295	0.0000	-577.8218	-576.1916	-576.8518	-576.3444	-577.3341	-577.0880	-577.1349
7c(iii) [product]	424.0717	0.0120	0.2933	-0.3389	0.0000	-523.2125	-521.6045	-522.2334	-521.7830	-522.7508	-522.4455	-522.4936
7c(iv) [product]	427.9890	0.0122	0.3087	-0.3389	0.0000	-523.5955	-521.9926	-522.6163	-522.1740	-523.1365	-522.8156	-522.8642
8c(ii) [product]	422.1951	0.0117	0.2506	-0.3577	0.0000	-616.5579	-614.7849	-615.5125	-614.9497	-616.0350	-615.7727	-615.8206
8c(i) [product]	425.3680	0.0119	0.2650	-0.3577	0.0000	-617.1153	-615.3540	-616.0674	-615.5228	-616.5938	-616.3170	-616.3653
8c(iii) [product]	438.1996	0.0129	0.3234	-0.3671	0.0000	-562.5025	-560.7631	-561.4461	-560.9576	-562.0077	-561.6714	-561.7212
8c(iv) [product]	441.2920	0.0130	0.3388	-0.3671	0.0000	-562.8870	-561.1529	-561.8303	-561.3502	-562.3947	-562.0428	-562.0929
7d(ii) [product]	403.7248	0.0107	0.2211	-0.3295	0.0000	-577.2668	-575.6241	-576.2993	-575.7728	-576.7775	-576.5458	-576.5916
7d(i) [product]	407.6532	0.0109	0.2352	-0.3295	0.0000	-577.8246	-576.1942	-576.8548	-576.3469	-577.3369	-577.0908	-577.1371
7d(iii) [product]	420.1216	0.0118	0.2935	-0.3389	0.0000	-523.2119	-521.6049	-522.2344	-521.7829	-522.7513	-522.4459	-522.4936
7d(iv) [product]	421.9955	0.0119	0.3090	-0.3389	0.0000	-523.5959	-521.9933	-522.6176	-522.1742	-523.1374	-522.8165	-522.8644
8d(ii) [product]	422.8755	0.0117	0.2503	-0.3577	0.0000	-616.5638	-614.7904	-615.5182	-614.9553	-616.0408	-615.7788	-615.8268
8d(i) [product]	426.1672	0.0119	0.2646	-0.3577	0.0000	-617.1217	-615.3603	-616.0737	-615.5290	-616.6002	-616.3237	-616.3721
8d(iii) [product]	441.0964	0.0130	0.3227	-0.3671	0.0000	-562.5091	-560.7695	-561.4520	-560.9640	-562.0136	-561.6779	-561.7280
8d(iv) [product]	443.1971	0.0131	0.3384	-0.3671	0.0000	-562.8935	-561.1592	-561.8366	-561.3565	-562.4010	-562.0494	-562.0997
3a(ii)[product]	436.2847	0.0122	0.2081	-0.3765	0.0000	-726.4984	-724.5605	-725.3767	-724.7126	-725.9053	-725.6850	-725.7345
3a(i) [product]	439.3143	0.0124	0.2222	-0.3765	0.0000	-727.0462	-725.1205	-725.9223	-725.2764	-726.4548	-726.2202	-726.2701
3a(iii) [product]	450.9864	0.0133	0.2805	-0.3859	0.0000	-672.4372	-670.5336	-671.3043	-670.7153	-671.8719	-671.5781	-671.6293
3a(iv) [product]	455.3215	0.0135	0.2958	-0.3859	0.0000	-672.8092	-670.9113	-671.6768	-671.0957	-672.2472	-671.9379	-671.9896
5a(ii) [product]	449.3398	0.0130	0.2377	-0.4048	0.0000	-765.7925	-763.7239	-764.5928	-763.8918	-765.1654	-764.9147	-764.9657
5a(i) [product]	452.7427	0.0132	0.2520	-0.4048	0.0000	-766.3401	-764.2837	-765.1385	-764.4554	-765.7149	-765.4497	-765.5011
5a(iii) [product]	467.9378	0.0143	0.3101	-0.4142	0.0000	-711.7279	-709.6931	-710.5171	-709.8907	-711.1288	-710.8044	-710.8575
5a(iv) [product]	469.0869	0.0144	0.3258	-0.4142	0.0000	-712.1024	-710.0736	-710.8925	-710.2738	-711.5068	-711.1667	-711.2200
3b(ii) [product]	433.9076	0.0121	0.2083	-0.3765	0.0000	-726.4997	-724.5618	-725.3781	-724.7140	-725.9068	-725.6865	-725.7357
3b(i) [product]	437.7326	0.0123	0.2222	-0.3765	0.0000	-727.0470	-725.1212	-725.9233	-725.2773	-726.4559	-726.2214	-726.2711
3b(iii) [product]	451.4368	0.0133	0.2805	-0.3859	0.0000	-672.4382	-670.5344	-671.3054	-670.7163	-671.8732	-671.5793	-671.6306
3b(iv) [product]	455.0116	0.0135	0.2959	-0.3859	0.0000	-672.8094	-670.9112	-671.6769	-671.0959	-672.2475	-671.9380	-671.9897
5c(ii) [product]	451.1657	0.0130	0.2376	-0.4048	0.0000	-765.7968	-763.7279	-764.5970	-763.8962	-765.1700	-764.9193	-764.9705
5c(i) [product]	454.7581	0.0133	0.2518	-0.4048	0.0000	-766.3445	-764.2878	-765.1429	-764.4598	-765.7197	-765.4546	-765.5062
5c(iii) [product]	469.6055	0.0144	0.3099	-0.4142	0.0000	-711.7328	-709.6976	-710.5218	-709.8955	-711.1339	-710.8096	-710.8629
5c(iv) [product]	472.2381	0.0145	0.3256	-0.4142	0.0000	-712.1066	-710.0772	-710.8964	-710.2778	-711.5111	-711.1711	-711.2247

5b(ii) [product]	448.6312	0.0130	0.2378	-0.4048	0.0000	-765.7930	-763.7245	-764.5934	-763.8924	-765.1661	-764.9153	-764.9662
5b(i) [product]	451.9662	0.0132	0.2520	-0.4048	0.0000	-766.3401	-764.2837	-765.1385	-764.4554	-765.7150	-765.4498	-765.5011
5b(iii) [product]	467.3516	0.0143	0.3102	-0.4142	0.0000	-711.7280	-709.6931	-710.5171	-709.8906	-711.1287	-710.8043	-710.8573
5b(iv) [product]	468.5461	0.0144	0.3257	-0.4142	0.0000	-712.1020	-710.0731	-710.8920	-710.2732	-711.5063	-711.1663	-711.2195
5d(ii) [product]	451.3269	0.0131	0.2376	-0.4048	0.0000	-765.7971	-763.7283	-764.5972	-763.8966	-765.1703	-764.9196	-764.9708
5d(i) [product]	454.9978	0.0133	0.2518	-0.4048	0.0000	-766.3444	-764.2875	-765.1426	-764.4597	-765.7195	-765.4544	-765.5060
5d(iii) [product]	469.8925	0.0144	0.3099	-0.4142	0.0000	-711.7328	-709.6976	-710.5219	-709.8955	-711.1340	-710.8097	-710.8630
5d(iv) [product]	472.2806	0.0145	0.3255	-0.4142	0.0000	-712.1062	-710.0768	-710.8961	-710.2773	-711.5109	-711.1708	-711.2245
3c(ii)[product]	434.9174	0.0121	0.2081	-0.3765	0.0000	-726.4934	-724.5560	-725.3718	-724.7083	-725.9005	-725.6803	-725.7297
3c(i) [product]	437.4411	0.0123	0.2223	-0.3765	0.0000	-727.0487	-725.1231	-725.9247	-725.2791	-726.4573	-726.2227	-726.2724
3c(iii) [product]	449.3269	0.0133	0.2806	-0.3859	0.0000	-672.4396	-670.5362	-671.3067	-670.7180	-671.8745	-671.5806	-671.6316
3c(iv) [product]	451.4301	0.0134	0.2961	-0.3859	0.0000	-672.8207	-670.9230	-671.6881	-671.1074	-672.2585	-671.9489	-672.0002
5e(ii) [product]	448.1717	0.0129	0.2378	-0.4048	0.0000	-765.7864	-763.7181	-764.5867	-763.8865	-765.1598	-764.9091	-764.9600
5e(i) [product]	450.7812	0.0132	0.2521	-0.4048	0.0000	-766.3414	-764.2855	-765.1395	-764.4576	-765.7164	-765.4512	-765.5024
5e(iii) [product]	467.0908	0.0143	0.3103	-0.4142	0.0000	-711.7291	-709.6949	-710.5182	-709.8928	-711.1303	-710.8057	-710.8588
5e(iv) [product]	466.5479	0.0143	0.3260	-0.4142	0.0000	-712.1142	-710.0858	-710.9037	-710.2864	-711.5183	-711.1780	-711.2310
3d(ii) [product]	434.3097	0.0121	0.2079	-0.3765	0.0000	-726.4933	-724.5551	-725.3712	-724.7079	-725.9005	-725.6805	-725.7299
3d(i) [product]	436.3468	0.0123	0.2221	-0.3765	0.0000	-727.0470	-725.1217	-725.9231	-725.2781	-726.4560	-726.2216	-726.2712
3d(iii) [product]	450.6326	0.0133	0.2804	-0.3859	0.0000	-672.4385	-670.5352	-671.3057	-670.7172	-671.8736	-671.5799	-671.6311
3d(iv) [product]	451.1111	0.0134	0.2962	-0.3859	0.0000	-672.8179	-670.9199	-671.6846	-671.1048	-672.2554	-671.9458	-671.9971
5g(ii) [product]	451.9777	0.0131	0.2374	-0.4048	0.0000	-765.7931	-763.7247	-764.5930	-763.8933	-765.1663	-764.9159	-764.9672
5g(i) [product]	454.8821	0.0133	0.2517	-0.4048	0.0000	-766.3445	-764.2881	-765.1427	-764.4604	-765.7198	-765.4548	-765.5065
5g(iii) [product]	469.7716	0.0144	0.3099	-0.4142	0.0000	-711.7333	-709.6985	-710.5224	-709.8965	-711.1346	-710.8103	-710.8636
5g(iv) [product]	467.0140	0.0143	0.3259	-0.4142	0.0000	-712.1130	-710.0835	-710.9023	-710.2842	-711.5172	-711.1770	-711.2300
5f(ii) [product]	448.0713	0.0129	0.2378	-0.4048	0.0000	-765.7855	-763.7175	-764.5856	-763.8859	-765.1587	-764.9080	-764.9589
5f(i) [product]	450.5539	0.0131	0.2522	-0.4048	0.0000	-766.3412	-764.2851	-765.1391	-764.4573	-765.7160	-765.4507	-765.5019
5f(iii) [product]	467.2445	0.0143	0.3102	-0.4142	0.0000	-711.7288	-709.6945	-710.5177	-709.8924	-711.1299	-710.8053	-710.8584
5f(iv) [product]	466.5042	0.0143	0.3262	-0.4142	0.0000	-712.1141	-710.0858	-710.9038	-710.2863	-711.5185	-711.1779	-711.2309
5h(ii) [product]	451.9504	0.0131	0.2374	-0.4048	0.0000	-765.7924	-763.7241	-764.5923	-763.8926	-765.1657	-764.9152	-764.9665
5h(i) [product]	454.4105	0.0133	0.2517	-0.4048	0.0000	-766.3445	-764.2881	-765.1426	-764.4604	-765.7197	-765.4547	-765.5063
5h(iii) [product]	469.6375	0.0144	0.3098	-0.4142	0.0000	-711.7332	-709.6984	-710.5222	-709.8965	-711.1345	-710.8103	-710.8636
5h(iv) [product]	468.0122	0.0144	0.3259	-0.4142	0.0000	-712.1129	-710.0835	-710.9024	-710.2842	-711.5173	-711.1770	-711.2302

Table S15: Components of the G3(MP2)-CC calculation in hartrees unless stated otherwise for every transition state calculated

	Entropy(J/mol K)	TC	ZPVE	HLC	SO	M062X/6-31+G**	MP2/6-31G*	MP2/large	URCCSD(T)/6-31G*	E	H	G
7a(ii)[transition state]	422.1259	0.0116	0.2158	-0.3295	0.0000	-577.1911	-575.5493	-576.2340	-575.6916	-576.7056	-576.4782	-576.5262
7a(i) [transition state]	424.4256	0.0117	0.2299	-0.3295	0.0000	-577.7513	-576.1227	-576.7915	-576.2686	-577.2668	-577.0252	-577.0734
7a(iii) [transition state]	436.0413	0.0127	0.2881	-0.3389	0.0000	-523.1414	-521.5348	-522.1726	-521.7065	-522.6831	-522.3823	-522.4318
7a(iv) [transition state]	440.0009	0.0129	0.3035	-0.3389	0.0000	-523.5273	-521.9262	-522.5585	-522.1004	-523.0715	-522.7551	-522.8051
8a(ii) [transition state]	437.0786	0.0125	0.2453	-0.3577	0.0000	-616.4904	-614.7200	-615.4556	-614.8779	-615.9713	-615.7135	-615.7631
8a(i) [transition state]	441.4599	0.0127	0.2595	-0.3577	0.0000	-617.0491	-615.2899	-616.0115	-615.4518	-616.5311	-616.2589	-616.3090
8a(iii) [transition state]	456.1701	0.0138	0.3179	-0.3671	0.0000	-562.4357	-560.6988	-561.3897	-560.8863	-561.9443	-561.6126	-561.6644
8a(iv) [transition state]	458.2034	0.0139	0.3334	-0.3671	0.0000	-562.8232	-561.0920	-561.7770	-561.2821	-562.3341	-561.9868	-562.0389
7b(ii) [transition state]	413.0763	0.0113	0.2159	-0.3295	0.0000	-577.1944	-575.5558	-576.2371	-575.6976	-576.7083	-576.4811	-576.5280
7b(i) [transition state]	418.0044	0.0116	0.2300	-0.3295	0.0000	-577.7500	-576.1213	-576.7895	-576.2671	-577.2647	-577.0232	-577.0706
7b(iii) [transition state]	437.4907	0.0128	0.2881	-0.3389	0.0000	-523.1376	-521.5311	-522.1689	-521.7029	-522.6795	-522.3786	-522.4283
7b(iv) [transition state]	440.1001	0.0129	0.3036	-0.3389	0.0000	-523.5243	-521.9233	-522.5552	-522.0976	-523.0684	-522.7519	-522.8018
8b(ii) [transition state]	440.7055	0.0126	0.2451	-0.3577	0.0000	-616.4877	-614.7158	-615.4528	-614.8739	-615.9686	-615.7108	-615.7609
8b(i) [transition state]	442.8524	0.0127	0.2595	-0.3577	0.0000	-617.0469	-615.2879	-616.0094	-615.4496	-616.5289	-616.2566	-616.3069
8b(iii) [transition state]	456.3150	0.0138	0.3179	-0.3671	0.0000	-562.4342	-560.6970	-561.3879	-560.8845	-561.9425	-561.6109	-561.6627
8b(iv) [transition state]	459.0445	0.0139	0.3333	-0.3671	0.0000	-562.8215	-561.0900	-561.7748	-561.2801	-562.3319	-561.9847	-562.0368
7c(ii)[transition state]	423.0534	0.0116	0.2157	-0.3295	0.0000	-577.1896	-575.5479	-576.2310	-575.6907	-576.7032	-576.4759	-576.5240
7c(i) [transition state]	427.1246	0.0118	0.2299	-0.3295	0.0000	-577.7461	-576.1169	-576.7855	-576.2635	-577.2615	-577.0197	-577.0682
7c(iii) [transition state]	439.3353	0.0128	0.2882	-0.3389	0.0000	-523.1364	-521.5293	-522.1670	-521.7015	-522.6781	-522.3771	-522.4270
7c(iv) [transition state]	438.7396	0.0128	0.3038	-0.3389	0.0000	-523.5195	-521.9177	-522.5502	-522.0919	-523.0633	-522.7467	-522.7965
8c(ii) [transition state]	437.7738	0.0125	0.2455	-0.3577	0.0000	-616.4894	-614.7193	-615.4542	-614.8773	-615.9700	-615.7120	-615.7617
8c(i) [transition state]	443.1194	0.0128	0.2596	-0.3577	0.0000	-617.0454	-615.2862	-616.0073	-615.4484	-616.5272	-616.2548	-616.3051
8c(iii) [transition state]	457.7446	0.0138	0.3179	-0.3671	0.0000	-562.4329	-560.6957	-561.3861	-560.8836	-561.9411	-561.6093	-561.6613
8c(iv) [transition state]	459.5758	0.0140	0.3334	-0.3671	0.0000	-562.8173	-561.0859	-561.7704	-561.2765	-562.3281	-561.9807	-562.0329
7d(ii) [transition state]	418.5831	0.0115	0.2158	-0.3295	0.0000	-577.1915	-575.5510	-576.2335	-575.6933	-576.7053	-576.4780	-576.5255
7d(i) [transition state]	421.1689	0.0116	0.2303	-0.3295	0.0000	-577.7460	-576.1172	-576.7851	-576.2635	-577.2609	-577.0190	-577.0668
7d(iii) [transition state]	436.8858	0.0128	0.2884	-0.3389	0.0000	-523.1331	-521.5254	-522.1633	-521.6974	-522.6743	-522.3731	-522.4227
7d(iv) [transition state]	439.3774	0.0129	0.3037	-0.3389	0.0000	-523.5195	-521.9181	-522.5497	-522.0928	-523.0633	-522.7467	-522.7966

8d(ii) [transition state]	431.4941	0.0123	0.2458	-0.3577	0.0000	-616.4935	-614.7245	-615.4580	-614.8821	-615.9733	-615.7153	-615.7643
8d(i) [transition state]	442.9657	0.0128	0.2596	-0.3577	0.0000	-617.0458	-615.2866	-616.0077	-615.4487	-616.5276	-616.2552	-616.3055
8d(iii) [transition state]	456.8184	0.0138	0.3179	-0.3671	0.0000	-562.4312	-560.6936	-561.3845	-560.8813	-561.9394	-561.6077	-561.6596
8d(iv) [transition state]	459.6306	0.0140	0.3335	-0.3671	0.0000	-562.8183	-561.0871	-561.7715	-561.2776	-562.3291	-561.9816	-562.0338
3a(ii)[transition state]	450.2170	0.0129	0.2030	-0.3765	0.0000	-726.4238	-724.4856	-725.3114	-724.6305	-725.8328	-725.6169	-725.6680
3a(i) [transition state]	451.3469	0.0130	0.2171	-0.3765	0.0000	-726.9699	-725.0455	-725.8560	-725.1938	-726.3808	-726.1506	-726.2019
3a(iii) [transition state]	464.2897	0.0140	0.2754	-0.3859	0.0000	-672.3611	-670.4587	-671.2382	-670.6327	-671.7982	-671.5087	-671.5615
3a(iv) [transition state]	468.0797	0.0142	0.2907	-0.3859	0.0000	-672.7324	-670.8363	-671.6104	-671.0129	-672.1730	-671.8681	-671.9212
5a(ii) [transition state]	469.9569	0.0140	0.2322	-0.4048	0.0000	-765.7227	-763.6540	-764.5304	-763.8167	-765.0978	-764.8517	-764.9051
5a(i) [transition state]	465.7856	0.0139	0.2470	-0.4048	0.0000	-766.2676	-764.2136	-765.0763	-764.3773	-765.6448	-765.3839	-765.4368
5a(iii) [transition state]	483.3134	0.0151	0.3051	-0.4142	0.0000	-711.6551	-709.6223	-710.4540	-709.8125	-711.0584	-710.7381	-710.7930
5a(iv) [transition state]	485.2839	0.0152	0.3206	-0.4142	0.0000	-712.0286	-710.0023	-710.8290	-710.1950	-711.4358	-711.0999	-711.1550
3b(ii) [transition state]	440.1334	0.0126	0.2034	-0.3765	0.0000	-726.4320	-724.4978	-725.3196	-724.6417	-725.8401	-725.6241	-725.6740
3b(i) [transition state]	444.7700	0.0128	0.2174	-0.3765	0.0000	-726.9698	-725.0457	-725.8555	-725.1935	-726.3799	-726.1497	-726.2002
3b(iii) [transition state]	464.7917	0.0141	0.2754	-0.3859	0.0000	-672.3577	-670.4554	-671.2348	-670.6295	-671.7949	-671.5054	-671.5582
3b(iv) [transition state]	468.2698	0.0142	0.2907	-0.3859	0.0000	-672.7297	-670.8338	-671.6075	-671.0104	-672.1701	-671.8652	-671.9184
5c(ii) [transition state]	455.3549	0.0135	0.2334	-0.4048	0.0000	-765.7296	-763.6655	-764.5394	-763.8255	-765.1042	-764.8573	-764.9090
5c(i) [transition state]	469.7615	0.0140	0.2468	-0.4048	0.0000	-766.2664	-764.2120	-765.0753	-764.3758	-765.6438	-765.3830	-765.4363
5c(iii) [transition state]	485.1412	0.0152	0.3050	-0.4142	0.0000	-711.6545	-709.6213	-710.4538	-709.8112	-711.0578	-710.7376	-710.7927
5c(iv) [transition state]	486.5635	0.0152	0.3206	-0.4142	0.0000	-712.0294	-710.0032	-710.8298	-710.1953	-711.4361	-711.1003	-711.1555
5b(ii) [transition state]	465.6409	0.0138	0.2326	-0.4048	0.0000	-765.7225	-763.6549	-764.5320	-763.8156	-765.0975	-764.8511	-764.9040
5b(i) [transition state]	468.4717	0.0140	0.2468	-0.4048	0.0000	-766.2678	-764.2129	-765.0761	-764.3772	-765.6452	-765.3844	-765.4376
5b(iii) [transition state]	483.7813	0.0152	0.3050	-0.4142	0.0000	-711.6561	-709.6233	-710.4550	-709.8133	-711.0593	-710.7391	-710.7940
5b(iv) [transition state]	482.8494	0.0150	0.3210	-0.4142	0.0000	-712.0331	-710.0073	-710.8340	-710.1990	-711.4400	-711.1039	-711.1588
5d(ii) [transition state]	456.3523	0.0135	0.2334	-0.4048	0.0000	-765.7315	-763.6674	-764.5415	-763.8272	-765.1060	-764.8592	-764.9110
5d(i) [transition state]	467.3871	0.0140	0.2470	-0.4048	0.0000	-766.2673	-764.2125	-765.0754	-764.3769	-765.6446	-765.3836	-765.4367
5d(iii) [transition state]	484.2094	0.0151	0.3052	-0.4142	0.0000	-711.6547	-709.6215	-710.4542	-709.8114	-711.0583	-710.7380	-710.7930
5d(iv) [transition state]	486.8306	0.0152	0.3205	-0.4142	0.0000	-712.0293	-710.0024	-710.8292	-710.1951	-711.4360	-711.1002	-711.1555
3c(ii)[transition state]	449.7747	0.0129	0.2027	-0.3765	0.0000	-726.4155	-724.4777	-725.3022	-724.6233	-725.8243	-725.6087	-725.6597
3c(i) [transition state]	448.1861	0.0130	0.2173	-0.3765	0.0000	-726.9719	-725.0478	-725.8574	-725.1963	-726.3823	-726.1521	-726.2030
3c(iii) [transition state]	461.2774	0.0140	0.2757	-0.3859	0.0000	-672.3621	-670.4603	-671.2389	-670.6344	-671.7990	-671.5094	-671.5618
3c(iv) [transition state]	460.4831	0.0140	0.2914	-0.3859	0.0000	-672.7475	-670.8522	-671.6250	-671.0284	-672.1871	-671.8818	-671.9341
5e(ii) [transition state]	465.2953	0.0138	0.2327	-0.4048	0.0000	-765.7194	-763.6532	-764.5290	-763.8139	-765.0945	-764.8480	-764.9008

5e(i) [transition state]	463.8076	0.0139	0.2472	-0.4048	0.0000	-766.2705	-764.2168	-765.0787	-764.3806	-765.6472	-765.3862	-765.4389
5e(iii) [transition state]	480.7046	0.0151	0.3053	-0.4142	0.0000	-711.6568	-709.6249	-710.4556	-709.8150	-711.0599	-710.7395	-710.7941
5e(iv) [transition state]	479.5325	0.0151	0.3213	-0.4142	0.0000	-712.0446	-710.0190	-710.8440	-710.2116	-711.4508	-711.1145	-711.1689
3d(ii) [transition state]	449.8766	0.0130	0.2026	-0.3765	0.0000	-726.4070	-724.4701	-725.2942	-724.6158	-725.8164	-725.6009	-725.6520
3d(i) [transition state]	443.4215	0.0129	0.2172	-0.3765	0.0000	-726.9678	-725.0439	-725.8525	-725.1921	-726.3772	-726.1472	-726.1975
3d(iii) [transition state]	461.4205	0.0140	0.2757	-0.3859	0.0000	-672.3560	-670.4547	-671.2324	-670.6290	-671.7925	-671.5028	-671.5552
3d(iv) [transition state]	454.0933	0.0138	0.2908	-0.3859	0.0000	-672.7605	-670.8663	-671.6381	-671.0421	-672.1998	-671.8952	-671.9468
5g(ii) [transition state]	465.3002	0.0138	0.2325	-0.4048	0.0000	-765.7141	-763.6472	-764.5233	-763.8080	-765.0889	-764.8425	-764.8954
5g(i) [transition state]	464.2484	0.0139	0.2471	-0.4048	0.0000	-766.2692	-764.2149	-765.0768	-764.3791	-765.6458	-765.3848	-765.4375
5g(iii) [transition state]	480.9272	0.0151	0.3052	-0.4142	0.0000	-711.6545	-709.6219	-710.4538	-709.8116	-711.0577	-710.7375	-710.7921
5g(iv) [transition state]	473.4211	0.0148	0.3207	-0.4142	0.0000	-712.0600	-710.0355	-710.8598	-710.2272	-711.4657	-711.1302	-711.1839
5f(ii) [transition state]	467.5700	0.0139	0.2325	-0.4048	0.0000	-765.7188	-763.6511	-764.5269	-763.8135	-765.0941	-764.8477	-764.9008
5f(i) [transition state]	463.5377	0.0138	0.2472	-0.4048	0.0000	-766.2700	-764.2162	-765.0781	-764.3803	-765.6469	-765.3859	-765.4386
5f(iii) [transition state]	478.7347	0.0150	0.3057	-0.4142	0.0000	-711.6569	-709.6248	-710.4563	-709.8148	-711.0605	-710.7399	-710.7942
5f(iv) [transition state]	474.7646	0.0149	0.3218	-0.4142	0.0000	-712.0492	-710.0233	-710.8481	-710.2153	-711.4543	-711.1176	-711.1715
5h(ii) [transition state]	470.4658	0.0140	0.2321	-0.4048	0.0000	-765.7111	-763.6440	-764.5207	-763.8050	-765.0865	-764.8404	-764.8938
5h(i) [transition state]	463.0444	0.0139	0.2471	-0.4048	0.0000	-766.2676	-764.2135	-765.0752	-764.3779	-765.6443	-765.3834	-765.4360
5h(iii) [transition state]	483.3464	0.0151	0.3050	-0.4142	0.0000	-711.6543	-709.6221	-710.4538	-709.8118	-711.0576	-710.7375	-710.7924
5h(iv) [transition state]	470.3685	0.0147	0.3210	-0.4142	0.0000	-712.0592	-710.0341	-710.8591	-710.2258	-711.4649	-711.1293	-711.1827

Gaussian Archive Entries:

1

1\1\GINC-R684\FOpt\RM062X\6-31+G(d,p)\C5H6\ROOT\29-Jun-2017\0\# M062X
/6-31+G** SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=671088
640\A-11.M062X\0,1\C,-4.3668099798,0.4347172852,0.6998708913\C,-3.17
33620203,0.0680566275,-0.0768554233\C,-3.9846918612,0.8996509765,1.904
6227757\C,-2.4852553877,0.8663306194,1.9953734663\C,-2.0734322074,0.31
24584509,0.6607263365\H,-5.3863487312,0.3398126322,0.3447444483\H,-3.1
925389247,-0.3341872184,-1.0830428234\H,-4.6325216238,1.2482212102,2.6
994817176\H,-2.1399660231,0.2338221992,2.824495422\H,-2.0641331513,1.8
656577882,2.1706907104\H,-1.0450223257,0.1460408919,0.3646458444\Version=ES64L-G09RevE.01\State=1-A\HF=-194.0195363\RMSD=8.647e-09\RMSF=3.
259e-05\Dipole=0.117445,0.0562114,0.1539204\Quadrupole=1.13467,-2.1199
073,0.9852373,0.0732969,0.6272164,1.4456453\PG=C02V [C2(C1),SGV(C4H4),
SGV'(H2)]\@

6

1\1\GINC-R212\FOpt\RM062X\6-31+G(d,p)\C5H4O2\ROOT\29-Jun-2017\0\# M06
2X/6-31+G** SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=6710
88640\B-30.M062X\0,1\C,-1.8364235972,2.1175803397,0.0739203317\C,-2.
9356005739,1.3337768676,-0.0091589603\C,-2.8071912174,-0.0978882086,-0
.0129524087\C,-1.5660527009,-0.6147235204,0.0684332788\O,-0.4589983107
,0.1442399015,0.1518380551\H,-1.8790114652,3.1994273281,0.0805579759\H
, -3.9219657421,1.7832057631,-0.0734954472\H,-3.6661701822,-0.751848996
8,-0.0782440009\H,-1.328917112,-1.6720079091,0.07548842\C,-0.503174442
7,1.5359802306,0.1611119971\O,0.5397153158,2.1300482006,0.2386111682\Version=ES64L-G09RevE.01\State=1-A\HF=-343.2405385\RMSD=5.462e-09\RMS
F=1.157e-04\Dipole=-1.7919954,-0.740873,-0.1306861\Quadrupole=-2.42489
87,3.4436803,-1.0187815,-2.6089944,-0.1211822,-0.1412475\PG=CS [SG(C5H
4O2)]\@

2(ii)

1\1\GINC-R265\FOpt\RM062X\6-31+G(d,p)\C6H7O2(1-)\ROOT\07-Aug-2017\0\#
M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=1
073741824\A5\1,1\C,-0.0575082556,1.1875852124,-0.2250982241\C,0.048
779973,0.042645449,0.4570654937\C,-0.2836999695,0.9460156059,-1.698343
3152\C,-0.5887034127,-0.5680115406,-1.7787443159\C,-0.0879770541,-1.16
28313812,-0.4418710606\H,0.0542374053,2.1783814254,0.2120894688\H,0.61
0933147,1.179702096,-2.2904129237\H,-1.0895869202,1.5589430588,-2.1169
252136\H,0.8751528161,-1.6675641071,-0.5940119118\H,-0.7663017918,-1.9
243609334,-0.0414936841\H,-1.6797503726,-0.6939758444,-1.8202150696\H,
0.2585421193,-0.0225057268,1.5233920195\C,-0.0348885716,-1.2754751479,
-3.05232985\O,0.0505286561,-0.5547160523,-4.075392835\O,0.2300702313,-
2.4943551134,-2.9198025784\Version=ES64L-G09RevE.01\State=1-A\HF=-383
.19807\RMSD=5.788e-09\RMSF=1.957e-06\Dipole=-0.4730696,1.6650263,2.868
1152\Quadrupole=8.4660229,-0.7794522,-7.6865707,1.8562234,2.1995652,-5
.9060647\PG=C01 [X(C6H7O2)]\@

4(ii)

1\1\GINC-R1245\FOpt\RM062X\6-31+G(d,p)\C7H9O2(1-)\ROOT\07-Aug-2017\0\#
M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=
1073741824\A4\1,1\C,-0.1652740039,1.1687550851,-0.2506007097\C,0.03
24542684,-0.0156797624,0.3397232011\C,-0.2092499873,1.3633647384,-1.74
45085126\C,0.3115614107,0.1474025181,-2.5087173104\C,-0.2498764243,-1.
135853382,-1.8944480833\C,0.1940873941,-1.2993769592,-0.437717119\H,-0
.2992149465,2.0505252821,0.3784596832\H,0.3613973164,2.2550971229,-2.0
27389695\H,-1.2358896929,1.5761284117,-2.0730801072\H,0.0603065982,-1.
9844207862,-2.5096298423\H,1.2485874847,-1.6147178952,-0.4034873507\H,
-0.3750096409,-2.1000907673,0.0554976537\H,1.4080759151,0.1073988968,-
2.3997437268\H,-1.3487219783,-1.0889241096,-1.9323204089\H,0.074991059
5,-0.0723464097,1.4280417079\C,0.0343732459,0.2177955929,-4.0484100622
\O,-0.4236854159,1.3016683087,-4.4808701821\O,0.3222133971,-0.82608788
49,-4.6813571356\Version=ES64L-G09RevE.01\State=1-A\HF=-422.5036004\R
MSD=2.718e-09\RMSF=2.047e-06\Dipole=0.1182128,-0.2499431,3.8196507\Qua
drupole=9.8304639,5.3184502,-15.1489141,1.9690179,-0.4020645,0.6128285
\PG=C01 [X(C7H9O2)]\@

2(i)

1\1\GINC-R1515\FOpt\RM062X\6-31+G(d,p)\C6H8O2\ROOT\07-Aug-2017\0\#M06
2X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=1073
741824\|a6\|0,1\C,-0.0829467354,1.1864137628,-0.2492241083\C,0.0551506
127,0.055706068,0.4441465805\C,-0.2969872058,0.9268434529,-1.720989406
4\C,-0.6080316553,-0.5976282043,-1.7485600152\C,-0.038398727,-1.167240
6373,-0.4365904675\H,-0.0056462891,2.187107139,0.1631721772\H,0.613359
8052,1.1624551268,-2.2891888427\H,-1.1073274295,1.5143032743,-2.160560
9772\H,0.9501756466,-1.6114002654,-0.6049744394\H,-0.675994328,-1.9523
674126,-0.0194510939\H,-1.6967557721,-0.7163377187,-1.7664901774\H,0.2
566888803,-0.0006198911,1.5088300181\C,-0.0658784937,-1.253546197,-2.9
911447424\O,0.8420030816,-2.0469901298,-3.0482603962\O,-0.7111436318,-
0.8218843423,-4.096549244\H,-0.3012437584,-1.2585440252,-4.8590508652\
\Version=ES64L-G09RevE.01\State=1-A\HF=-383.7573989\RMSD=7.791e-09\RM
SF=1.026e-05\Dipole=-0.4162406,0.4476729,0.0154595\Quadrupole=-2.774013
7,-1.3221911,4.0962048,2.5428251,0.6000426,-0.2257861\PG=C01 [X(C6H8O2
)]\@

4(i)

1\1\GINC-R1313\FOpt\RM062X\6-31+G(d,p)\C7H10O2\ROOT\07-Aug-2017\0\#M0
62X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=107
3741824\|a5\|0,1\C,0.0854895114,1.1992030373,-0.2769490401\C,0.1205117
567,0.0058459767,0.3212527036\C,-0.0352439417,1.3844359274,-1.76695804
\C,0.2448578107,0.0821195683,-2.5140820536\C,-0.5054640656,-1.08972099
64,-1.8539830875\C,0.000724167,-1.2974172608,-0.4258597565\H,0.1525552
22,2.1010825556,0.3273516349\H,0.6563116381,2.1648966411,-2.10382587\H
, -1.0382024306,1.744047546,-2.0293956529\H,-0.3805374616,-2.0018759714
, -2.4440602332\H,0.9766177934,-1.8027589828,-0.4429745978\H,-0.6772191
372,-1.9693906277,0.1125123367\H,1.3185088558,-0.1476275728,-2.4795164
672\H,-1.5757943488,-0.8475299126,-1.8335081496\H,0.2355039505,-0.0465
791196,1.4016622726\C,-0.1353561509,0.1932479579,-3.9710601598\O,-0.79
54963773,1.0724008805,-4.4703247353\O,0.3389859182,-0.8441444939,-4.69
4298145\H,0.0393512897,-0.7189891527,-5.6077949593\Version=ES64L-G09R
evE.01\State=1-A\HF=-423.0618899\RMSD=4.766e-09\RMSE=2.765e-06\Dipole=
0.2914464,-0.5600793,0.2512778\Quadrupole=-1.692386,-0.6674408,2.35982
69,2.0338422,-1.2859936,2.6509852\PG=C01 [X(C7H10O2)]\@

2(iii)

1\1\GINC-R2696\FOpt\RM062X\6-31+G(d,p)\C7H13N1\ROOT\07-Aug-2017\0\#M0
62X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=107
3741824\|a3\|0,1\C,-0.121295449,-0.9431553326,1.0964146256\C,0.0830007
962,0.3705951902,1.2197389281\C,0.0340772074,-1.664781243,2.4124836606
\C,0.0004023127,-0.4964919119,3.4415987381\C,0.410553007,0.7590710299,
2.6394429544\H,-0.3416326771,-1.4523105377,0.1631925803\H,0.9895038687
, -2.2069896787,2.4415746738\H,-0.75455949,-2.4025561632,2.5937397941\H
, -1.4804011809,0.9807066393,2.7413767256\H,-0.1258863664,1.6469427825,2
.9873448687\H,-1.0512638824,-0.3546751664,3.7203154316\N,0.7229562694,
-0.6677263503,4.6966095678\C,2.1349913849,-0.9809337701,4.5572045678\H
, 2.6148889044,-0.8942636939,5.5366034329\H,2.3200436501,-2.0033840412,
4.1816094199\H,2.6248452402,-0.2772599462,3.8812649876\C,0.0781097473,
-1.6405148554,5.5617311789\H,0.1155353867,-2.6687096581,5.1555198415\H
, 0.5735977263,-1.6467942424,6.5372083664\H,-0.9700480901,-1.3666645988
, 5.7121082484\H,0.0541072728,1.0829055479,0.4012894078\Version=ES64L-
G09RevE.01\State=1-A\HF=-329.1451049\RMSD=6.845e-09\RMSE=3.312e-06\Dip
ole=0.0482937,-0.2454727,-0.0492342\Quadrupole=0.0873773,0.0378625,-0.
1252398,0.3319884,0.029198,-1.407696\PG=C01 [X(C7H13N1)]\@

4(iii)

1\1\GINC-R1406\FOpt\RM062X\6-31+G(d,p)\C8H15N1\ROOT\07-Aug-2017\0\#M0
62X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=107
3741824\|a2\|0,1\C,0.3374003657,-1.4648082735,0.834082152\C,0.54630539
86,-0.1867022828,0.5071380121\C,0.4572334399,-1.9953726876,2.241306889
8\C,1.1809030695,-0.9934205216,3.1581817277\C,0.5935211492,0.401972919
1,2.9443695657\C,0.87683194,0.8805851809,1.5188503494\H,0.0810762225,-
2.1787737236,0.0538116222\H,0.9957042943,-2.9505004709,2.2205083241\H,
-0.5443531241,-2.2169009922,2.637619582\H,1.0132680337,1.0915662676,3.

6841531919\H,1.9333169505,1.1668239977,1.4183110294\H,0.2976660679,1.7854976621,1.3018166237\H,2.2308830198,-0.9524134914,2.8307266723\H,-0.4938540198,0.3724593887,3.0916351486\N,1.2298985793,-1.3558142662,4.5770593598\C,1.9628220845,-2.5862070256,4.8158445688\H,2.158108862,-2.6890932218,5.8877423341\H,1.4233697654,-3.4919205812,4.4838277129\H,2.9248707096,-2.5492197871,4.2957537002\C,-0.055226237,-1.383918397,5.2539595739\H,-0.7241798107,-2.1900381654,4.9015645306\H,0.1158294473,-1.5411129175,6.3231745993\H,-0.5716477081,-0.4287447904,5.1385492886\H,0.4723815001,0.1153871796,-0.5355955591\Version=ES64L-G09RevE.01\State=1-A\HF=-368.4497464\RMSD=6.726e-09\RMSF=7.369e-06\Dipole=-0.1131697,-0.1299579,-0.052214\Quadrupole=-0.8319918,1.1929718,-0.36098,-0.5280495,-0.8755441,-1.2705276\PG=C01 [X(C8H15N1)]\@

2(iv)

1\1\GINC-R439\FOpt\RM062X\6-31+G(d,p)\C7H14N1(1+)\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=1073741824\|a2\|1,1\C,0.4352178961,-1.163547166,1.2805397396\C,-0.092904625,0.053928791,1.3984049452\C,-0.5254497326,-2.2430240396,1.7229675683\C,-1.6559787244,-1.455908059,2.4149773635\C,-1.5003923828,0.0053775171,1.9447744608\H,1.4118190436,-1.3889837109,0.8676582707\H,-0.0650214177,-3.0058567241,2.3603346919\H,-0.9316856665,-2.7817175665,0.8596488139\H,-1.6908794703,0.7342261931,2.7442179979\H,-2.2334677074,0.222388652,1.160051521\N,-1.5531219788,-1.5322598251,3.938764568\C,-1.9355457698,-2.8799558954,4.4654444134\H,-1.9476888503,-2.8402421826,5.5545601365\H,-2.9232295102,-3.1415461185,4.0864832506\C,-0.2341324863,-1.0913351805,4.4963776211\H,0.536739698,-1.7834334815,4.1599778562\H,-0.0086028535,-0.0869525708,4.1432139951\H,-0.302329486,-1.107424565,5.5840539458\H,-2.2542262618,-0.870142864,4.2865260207\H,-2.6468230708,-1.8606830699,2.1995947718\H,0.3831337588,0.9798107157,1.0966427671\H,-1.2002754023,-3.6108938496,4.1313372809\Version=ES64L-G09RevE.01\State=1-A\HF=-329.5270252\RMSD=6.197e-09\RMSF=5.096e-06\Dipole=-0.7955461,-0.3701597,1.3996817\Quadrupole=-1.4441642,-0.9914832,2.4356474,0.957111,-2.7754356,-2.1089898\PG=C01 [X(C7H14N1)]\@

4(iv)

1\1\GINC-R2435\FOpt\RM062X\6-31+G(d,p)\C8H16N1(1+)\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=1073741824\|a4\|1,1\C,0.0953877177,-0.5431495938,0.1386572375\C,-0.4516842728,0.677311524,0.0993478846\C,1.33287537,-0.8565354818,0.9492750041\C,2.1374912254,0.4177793039,1.2035622313\C,1.2127224762,1.4616403873,1.8363809778\C,0.077782877,1.8560971062,0.8799080155\H,-0.3607892453,-1.3579796474,-0.4159924019\H,1.9309623777,-1.6392408619,0.4768352991\H,1.0545437644,-1.263195643,1.9285515873\H,1.7579251331,2.3373661064,2.195810502\H,0.392841746,2.6508449397,0.185569455\H,-0.7382901557,2.3048241067,1.4546954282\N,2.6984764877,0.949581092,-0.1181085447\C,3.4443227357,2.2339710733,0.0546417637\H,3.8281856404,2.5487340524,-0.9150962239\H,2.7787596344,2.9973831157,0.4502146167\H,4.2717448579,2.0587021018,0.7444007135\C,3.5551470021,-0.0497338799,-0.8311388392\H,2.9407951581,-0.87657413,-1.1794001714\H,4.0235985416,0.4394137812,-1.6843636284\H,4.3196155002,-0.405712462,-0.1385364881\H,1.8784981565,1.1246227661,-0.7143492801\H,3.0177571302,0.2237752126,1.8246758786\H,0.7889091789,0.9848031046,2.7251228058\H,-1.3392330376,0.8452729258,-0.5050208231\Version=ES64L-G09RevE.01\State=1-A\HF=-368.8339038\RMSD=3.641e-09\RMSF=5.074e-06\Dipole=1.3584775,0.3166589,-0.5123243\Quadrupole=3.0114261,-0.6338075,-2.3776186,0.5486002,-2.8241426,0.3340925\PG=C01 [X(C8H16N1)]\@

7a(ii)[product]

1\1\GINC-R739\FOpt\RM062X\6-31+G(d,p)\C11H13O2(1-)\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=1610612736\|a1\|1,1\C,1.1422214308,-0.0531530349,1.1444604485\C,1.012826343,1.0870796072,0.083492818\C,1.3248971952,-1.3583672068,0.3489584882\C,1.1247528019,0.4054526479,-1.2922130929\C,-0.1658911652,0.117752147,1.9932200854\C,-0.3521025404,1.7587871416,0.4663012709\C,-1.4528523211,0.7517764031,0.1885678818\C,-1.3419711027,-0.2253043476,1.0976602113\C,-0.277629319,1.6571103525,2.0045983225\H,0.8066079526,-2.207517

4071,0.8127328227\H,2.3909018202,-1.605608713,0.2905357793\H,0.4588987
853,0.8571156734,-2.038810621\H,2.1528599954,0.4923528878,-1.661472775
7\H,-2.0905256267,0.7498839361,-0.6890285943\H,-1.8724808148,-1.171543
9185,1.0986912536\H,0.6079006764,2.1486861294,2.4249421498\H,-1.184252
1103,2.0173837435,2.5023647416\H,-0.1367801477,-0.3895597129,2.9611599
475\H,-0.4934789617,2.7538877374,0.0362956132\C,0.8464690342,-1.098276
459,-1.0937737772\H,-0.2195751451,-1.3131159426,-1.1946465547\H,1.9930
081147,0.1230972359,1.8142486315\H,1.7979029536,1.8420018563,0.2148865
784\C,1.6093603189,-1.9807941466,-2.1353557747\O,2.8580061364,-1.84268
63792,-2.1387133357\O,0.8971856963,-2.7251602309,-2.8491325182\Version
=ES64L-G09RevE.01\State=1-A\HF=-577.2623297\RMSD=2.964e-09\RMSF=5.895
e-06\Dipole=-1.9868241,3.3087653,3.7985197\Quadrupole=4.3892914,0.4802
697,-4.8695611,9.1777381,11.5356447,-20.0792943\PG=C01 [X(C11H13O2)]\@

7a(i) [product]

1\1\GINC-R3403\FOpt\RM062X\6-31+G(d,p)\C11H14O2\ROOT\07-Aug-2017\0\#M
062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=16
10612736\|a2\0,1\C,1.1917265754,0.0363688859,1.1488619174\C,0.9773674
027,1.1543110499,0.0774442373\C,1.4426147691,-1.2732655083,0.381714244
7\C,1.1019445374,0.4788860033,-1.299194471\C,-0.1131462119,0.128062597
1,2.0093955969\C,-0.4204325927,1.7415374356,0.4712468746\C,-1.46309818
22,0.6666227821,0.2179316334\C,-1.2796135612,-0.2945083854,1.132680377
7\C,-0.31693847,1.6580786088,2.0088333514\H,0.9591843707,-2.1404424682
,0.8421906089\H,2.5188281017,-1.4791682152,0.3490710963\H,0.3759090564
,0.8635571313,-2.023516697\H,2.0975970507,0.6490634899,-1.7202576445\H
,-2.1505380516,0.6471345233,-0.6211948154\H,-1.7873699026,-1.251821708
7,1.1861842289\H,0.5388190488,2.2086172116,2.4152370243\H,-1.236490817
9,1.9640287325,2.5143797269\H,-0.0383961703,-0.3679564769,2.97909443\H
, -0.6261491351,2.720722571,0.0346033907\C,0.927305309,-1.0276690818,-1
.0614664488\H,-0.1240649601,-1.3193669311,-1.1183667978\H,2.0423677804
,0.2645699477,1.7987100246\H,1.7196069067,1.9519916052,0.1807679106\C,
1.6825538286,-1.8819473202,-2.0468181762\O,2.5344586775,-1.5109868835,
-2.8185771675\O,1.3238694508,-3.1817360016,-1.9523634125\H,1.869933189
9,-3.676261594,-2.5827480441\Version=ES64L-G09RevE.01\State=1-A\HF=-5
77.8231698\RMSD=8.083e-09\RMSF=6.021e-06\Dipole=-0.3191096,-0.0843751,
0.549896\Quadrupole=-2.4134443,4.4766434,-2.0631991,-0.5161354,4.56532
28,1.2680468\PG=C01 [X(C11H14O2)]\@

7a(iii) [product]

1\1\GINC-R1248\FOpt\RM062X\6-31+G(d,p)\C12H19N1\ROOT\07-Aug-2017\0\#M
062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=16
10612736\|a6\0,1\C,1.2249305014,0.250996964,1.1283193034\C,0.76664472
37,1.143511074,-0.0688433408\C,1.5680339864,-1.1267973881,0.5406495553
\C,0.8528438615,0.2656857581,-1.3271851138\C,0.0067574406,0.3392523975
,2.1095107184\C,-0.653448191,1.6251684969,0.3847811886\C,-1.5637713208
,0.4107081634,0.422145964\C,-1.1708715749,-0.3545673435,1.4486260715\C
, -0.3942992613,1.8141956714,1.8946016765\H,1.2472466223,-1.9444338945,
1.1960840678\H,2.6530131178,-1.2148551465,0.4060262764\H,0.0181999697,
0.4483918718,-2.0134884554\H,1.7819353132,0.4809837522,-1.8689399975\H
, -2.3130019773,0.167199123,-0.3236712774\H,-1.5373767513,-1.3435192912
,1.7026622836\H,0.417619285,2.5182299103,2.1087360877\H,-1.2933709637,
2.0959607682,2.4488407952\H,0.2373873691,0.0258929082,3.1297402955\H,-
1.0263825699,2.4873810853,-0.1717798904\C,0.9212406622,-1.2018883589,-
0.8575542189\H,-0.103508632,-1.6087890268,-0.7685327203\H,2.0957458784
,0.6797429142,1.6346210635\H,1.4036845289,2.0276457611,-0.1735628922\N
,1.6898974139,-2.0429482992,-1.7788865381\C,1.783932777,-3.4077127313,
-1.2829267232\H,2.3474186748,-4.0156473441,-1.9959769219\H,2.311734737
1,-3.4327431303,-0.327370644\H,0.7876183902,-3.8712539056,-1.143580279
5\C,1.086888372,-2.0506850697,-3.103168469\H,0.044062185,-2.423695318
9,-3.085287106\H,1.0854521494,-1.0454514148,-3.5295460734\H,1.67018081
73,-2.6971689561,-3.7645056853\Version=ES64L-G09RevE.01\State=1-A\HF=
-523.2130792\RMSD=7.124e-09\RMSF=3.989e-06\Dipole=-0.099048,-0.0146014
,0.0270753\Quadrupole=-2.6745433,1.8269074,0.8476359,0.6207064,2.23093
7,-0.3244145\PG=C01 [X(C12H19N1)]\@

7a(iv) [product]

1\1\GINC-R364\FOpt\RM062X\6-31+G(d,p)\C12H20N1(1+)\ROOT\08-Aug-2017\0
\\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk
=1610612736\|a6\|1,C,1.2394212203,0.2788089619,1.1017783396\C,0.7610
433227,1.1707305704,-0.0902226613\C,1.5864859708,-1.1002856098,0.51218
45435\C,0.8367590826,0.2974223183,-1.3557919305\C,0.0267030309,0.34284
1313,2.0883645834\C,-0.6624486237,1.6279069277,0.3711402218\C,-1.55814
7153,0.4005848363,0.4106681151\C,-1.1480606463,-0.3640303686,1.4322706
975\C,-0.3924058689,1.8142286575,1.8799474262\H,1.2869216512,-1.921899
7094,1.1698643564\H,2.6740264585,-1.1719568034,0.3655686171\H,-0.00028
69292,0.477817934,-2.0370917277\H,1.7640068057,0.524547435,-1.90165503
33\H,-2.3482024981,0.1788983874,-0.2994753052\H,-1.5363927578,-1.33476
54484,1.7229567238\H,0.4074537991,2.5304683568,2.094940594\H,-1.291426
677,2.0795195662,2.4392715099\H,0.2700357778,0.029342382,3.1043142612\H,
-1.0478506403,2.4868472839,-0.1796123513\C,0.8871931528,-1.154072217
,-0.8547769168\H,-0.1125344714,-1.58839836,-0.7785462777\H,2.115557448
2,0.7040902578,1.5975707153\H,1.3904032909,2.0561586841,-0.2094149715\H,
2.5735154892,-1.6788114996,-1.9243330303\N,1.6251569936,-2.059637916
9,-1.8286373815\C,1.7458276994,-3.4577122485,-1.3111350854\H,2.2743532
408,-4.0635854426,-2.0469378494\H,2.2917982606,-3.448539949,-0.3697865
934\H,0.7387164631,-3.8482361772,-1.1578391197\C,0.9938709511,-2.05568
7355,-3.1845041301\H,-0.0323386725,-2.4108169602,-3.0793689485\H,1.001
3066474,-1.0432031784,-3.5834375425\H,1.5554961814,-2.7221706283,-3.83
88908488\|Version=ES64L-G09RevE.01\|State=1-A\HF=-523.599176\|RMSD=3.651
e-09\|RMSF=1.448e-05\|Dipole=1.5178708,-2.2443924,-2.2886857\|Quadrupole=
-6.1958155,3.4917532,2.7040623,-5.9223472,-4.5494027,9.8459387\|PG=C01
[X(C12H20N1)]\|@

8a(ii) [product]

1\1\GINC-R1214\FOpt\RM062X\6-31+G(d,p)\C12H15O2(1-)\ROOT\07-Aug-2017\0
\\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdis
k=1610612736\|a2\|1,C,1.1355377853,0.0258822335,1.2784755227\C,0.97
09410841,1.1021958855,0.156804439\C,1.4234389283,-1.3800366751,0.74363
29721\C,0.5435113898,-1.8593140747,-0.4241827547\C,0.3679276823,-0.791
0857915,-1.5212167048\C,1.1145658648,0.5246722502,-1.2557135417\C,-0.1
535814295,0.2403008701,2.1478499637\C,-0.3857786966,1.794141782,0.5380
495103\C,-1.5157704639,0.7942936089,0.3717031557\C,-1.3742146918,-0.13
33946097,1.3275864907\C,-0.2554482143,1.7803946965,2.0772283512\H,1.36
33627137,-2.1217421078,1.5474996786\H,2.4690804178,-1.3908267265,0.401
8390854\H,-0.4359285501,-2.1300726551,-0.0158369338\H,-0.6981297912,-0
.5820970077,-1.667155068\H,0.818231263,1.2846731435,-1.9936252653\H,2.
1845602499,0.3422946107,-1.4238535467\H,-2.2192197377,0.777430331,-0.4
533415298\H,-1.9380597957,-1.0529523814,1.4342956498\H,0.6454431734,2.
2901304564,2.4403916981\H,-1.1437077115,2.1734164976,2.5820875673\H,-0
.0893040714,-0.2141163008,3.1397319652\H,-0.5317885431,2.7653935285,0.
0565954404\H,0.7480582434,-1.2245770233,-2.4518392463\H,1.9781425862,0
.3116360806,1.9236439878\H,1.7452460887,1.872081514,0.2807560885\C,1.1
679039474,-3.2091440441,-0.9344197306\O,1.7109412828,-3.1999193173,-2.
0639548283\O,1.078373996,-4.1518927739,-0.1115254163\|Version=ES64L-GO
9RevE.01\|State=1-A\HF=-616.5558319\|RMSD=9.036e-09\|RMSF=6.409e-06\|Dipol
e=-1.4288755,4.9305294,1.9689129\|Quadrupole=13.0899629,-20.0807837,6.9
908208,12.1197111,7.4297865,-12.7348774\|PG=C01 [X(C12H15O2)]\|@

8a(i) [product]

1\1\GINC-R3224\FOpt\RM062X\6-31+G(d,p)\C12H16O2\ROOT\07-Aug-2017\0\\#M
062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=16
10612736\|a2\|0,1,C,1.1476388221,0.0241964708,1.2756260585\C,0.9742091
699,1.0975070395,0.1540802146\C,1.4477378309,-1.3807314516,0.744842497
2\C,0.5495701185,-1.8372789113,-0.4303853423\C,0.3972920572,-0.7780625
253,-1.5423097255\C,1.1435933292,0.5318069735,-1.2585184208\C,-0.13977
01444,0.2220462806,2.1485507025\C,-0.3949427478,1.7633396802,0.5282760
107\C,-1.5105553853,0.7451897718,0.3692082423\C,-1.3612871263,-0.17013
2154,1.3354813813\C,-0.2612946933,1.7601680062,2.0678523408\H,1.379308
5172,-2.1138616993,1.5558798368\H,2.4906586514,-1.3926315628,0.4006639
987\H,-0.4315994453,-2.0911256483,-0.0193401198\H,-0.6666224711,-0.574
809807,-1.686825655\H,0.8454621593,1.2852940961,-1.9975987487\H,2.2154
182936,0.3595901259,-1.4206028361\H,-2.2411947261,0.7379412933,-0.4322
936247\H,-1.9468377086,-1.0715622667,1.4811166038\H,0.6294932775,2.287

1652398,2.4281347553\H,-1.1539070276,2.1396778675,2.5713503737\H,-0.06
50712752,-0.2231247239,3.1430294777\H,-0.5569025637,2.7277650765,0.042
0096002\H,0.7721587004,-1.1944812425,-2.4812814268\H,1.9957376259,0.30
25161393,1.9124067458\H,1.73586499,1.8755635585,0.2838171338\C,1.12508
18996,-3.1333401753,-0.9594091387\O,1.7042809584,-3.2946547653,-2.0068
54845\O,0.9526009721,-4.1472236269,-0.0816590855\H,1.3730999417,-4.931
9290594,-0.4653050046\Version=ES64L-G09RevE.01\State=1-A\HF=-617.1156
853\RMSD=4.308e-09\RMSF=1.119e-05\Dipole=-0.1259591,0.2353276,0.600332
1\Quadrupole=-0.3473591,4.0840522,-3.7366932,1.3019348,3.8994499,-3.30
85985\PG=C01 [X(C12H16O2)]\@

8a(iii) [product]

1\1\GINC-R1232\FOpt\RM062X\6-31+G(d,p)\C13H21N1\ROOT\07-Aug-2017\0\#M
062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=16
10612736\|a5\|1,C,1.2834627808,0.1829389686,1.0188900994\C,0.7862405
067,1.2082046788,-0.0499729782\C,1.6293727773,-1.19233127,0.4355454105
\C,0.5986702501,-1.7874808953,-0.5458170805\C,0.1075649204,-0.75666866
78,-1.5921437192\C,0.7451935743,0.6323195878,-1.4688992166\C,0.1707889
738,0.2654360647,2.1209475139\C,-0.5515736877,1.7343918677,0.576384619
8\C,-1.56024072,0.6007328578,0.635135751\C,-1.1320614876,-0.2719680652
,1.5563362788\C,-0.129118912,1.7800316597,2.0620297691\H,1.811004193,-
1.9012564559,1.2537297891\H,2.5860229513,-1.0850127391,-0.0922948938\H
, -0.2711433384,-2.1053518905,0.0371136482\H,-0.979502024,-0.6726757218
, -1.5155087874\H,0.2336868816,1.334348665,-2.1392924352\H,1.7818646508
,0.5742044598,-1.8288654395\H,-2.4220791075,0.4959878946,-0.0148166642
\H,-1.5752793934,-1.229590865,1.8072137255\H,0.7519227869,2.4057312115
,2.2446052084\H,-0.9459147884,2.0753145909,2.7254631037\H,0.4799664684
, -0.1463985427,3.0842183423\H,-0.9059204829,2.6653358932,0.1281791771\
H,0.3016747732,-1.1554143259,-2.5928943478\H,2.1987710142,0.5682726786
,1.4842772753\H,1.4696167017,2.0658235942,-0.0683114088\N,1.0600748734
, -3.0139459308,-1.2175870861\C,1.1241757271,-4.1644105955,-0.335755288
\H,0.173495905,-4.2786936081,0.1934111135\H,1.2922506827,-5.0671672683
, -0.931906121\H,1.9351900895,-4.1035198756,0.4131612248\C,2.2981427949
, -2.8744750185,-1.9646693669\H,2.4066386855,-3.7270147226,-2.642791835
5\H,2.2782696714,-1.9638442406,-2.5704685027\H,3.1971303078,-2.8402949
739,-1.323701879\Version=ES64L-G09RevE.01\State=1-A\HF=-562.5024294\R
MSD=4.238e-09\RMSF=8.213e-06\Dipole=0.28472,0.1492234,0.1449096\Quadr
pole=0.0661904,0.7367874,-0.8029779,-0.1588885,0.0215413,-2.043009\PG=
C01 [X(C13H21N1)]\@

8a(iv) [product]

1\1\GINC-R159\FOpt\RM062X\6-31+G(d,p)\C13H22N1(1+)\ROOT\07-Aug-2017\0\
\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk
=16\10612736\|a3\|1,C,1.0726167742,-0.0046149163,1.2921495822\C,0.981
5049699,1.1009294743,0.195840275\C,1.349792199,-1.413118221,0.73964380
46\C,0.4781596165,-1.7921356684,-0.4593655086\C,0.4620863012,-0.719477
2395,-1.5737096213\C,1.223894334,0.5659651225,-1.2150954389\C,-0.24902
02996,0.2015636755,2.1096878802\C,-0.3918695925,1.7826711382,0.5112321
917\C,-1.5176341568,0.7902611572,0.2736246179\C,-1.4391081658,-0.14555
45979,1.229528444\C,-0.3335449868,1.7437560432,2.0557315716\H,1.218006
3688,-2.1345765707,1.5522758219\H,2.4061630749,-1.4568247872,0.4340104
265\H,-0.5391060448,-2.0102269638,-0.1246143261\H,-0.5759993288,-0.489
1434981,-1.8237696402\H,0.9805307892,1.3321195486,-1.9583948893\H,2.29
91199869,0.3755941573,-1.3224459161\H,-2.2310442784,0.837484084,-0.542
5565845\H,-2.0814948806,-1.0114608479,1.3563322968\H,0.5452190295,2.24
65365495,2.472992829\H,-1.2420860375,2.1285108962,2.5226827156\H,-0.23
06078404,-0.2637178629,3.0969065292\H,-0.5105892739,2.7592123779,0.039
4888617\H,0.915099767,-1.1191029991,-2.4908317285\H,1.9038695764,0.216
7408438,1.9690108287\H,1.7515850789,1.8559412824,0.3837384962\N,0.9455
938008,-3.1254110905,-1.0642299729\H,1.8223846951,-2.9303843767,-1.559
9997747\C,-0.0446453128,-3.6391268972,-2.0633818969\H,-0.2817614988,-2
.8590491394,-2.7834287163\H,0.3798568254,-4.5042489363,-2.5723848356\H
, -0.9442144517,-3.9301028201,-1.5192919075\C,1.2266156752,-4.189459607
3,-0.0509106376\H,1.4281480744,-5.1231059782,-0.5758805693\H,2.0875753
23,-3.9087828804,0.5509305966\H,0.3434398887,-4.3002804517,0.580329194
9\Version=ES64L-G09RevE.01\State=1-A\HF=-562.8899312\RMSD=3.102e-09\R
MSF=6.537e-06\Dipole=0.9091414,-3.2093982,-1.5453118\Quadrupole=-9.179

3132,12.9533715,-3.7740582,-3.6659243,-0.4025488,8.5987536\PG=C01 [X(C13H22N1)]\@

7b(ii) [product]

1\1\GINC-R2430\FOpt\RM062X\6-31+G(d,p)\C11H13O2(1-)\ROOT\07-Aug-2017\0\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdis k=1610612736\|a4\|0,1\C,1.4739139874,0.0490309554,1.112278493\C,1.3617958203,1.1592172482,0.0096890773\C,1.5777967348,-1.2784213535,0.346304607\C,1.4072853546,0.4099704741,-1.3305337494\H,1.1208373753,-2.1172652948,0.8825950669\H,2.622302973,-1.535111154,0.134785495\H,0.8162511785,0.8987260407,-2.1127581867\H,2.4364041629,0.3056459339,-1.6933755038\C,2.6839585389,0.5423126511,1.975386298\C,2.5226620422,2.1394593425,0.3891686977\C,3.8312257676,1.4024773302,0.1670469142\C,3.9269138528,0.4549805661,1.1080600669\C,2.4349410078,2.0670223982,1.9305378414\H,2.7555481985,0.0797468578,2.9631304267\H,2.4474843279,3.1301738773,-0.0664228715\H,4.4809598227,1.526177037,-0.6922418876\H,4.6688584122,-0.3343817266,1.1555852863\H,3.2163474045,2.6462085774,2.4342563573\H,1.4474404478,2.3496781199,2.3155562849\C,0.9058844943,-1.0096282369,-1.0118270163\H,-0.1865935047,-1.010426104,-0.9015404055\H,0.5781884981,0.0540923728,1.7468751716\H,0.4119743743,1.6999330658,0.1122967772\C,1.2933980581,-2.0543959055,-2.1031979638\O,0.3438698187,-2.677064044,-2.6336023538\O,2.5258854335,-2.1511003718,-2.3258957287\Version=ES64L-G09RevE.01\State=1-A\HF=-577.2626395\RMSD=3.898e-09\RMSF=2.726e-05\Dipole=1.4118967,3.746606,3.6288498\Quadrupole=-105.5480422,43.2395739,62.3084683,-97.662451,-85.7666941,35.289753\PG=CS [SG(C3H3O2),X(C8H10)]\@

7b(i) [product]

1\1\GINC-R206\FOpt\RM062X\6-31+G(d,p)\C11H14O2\ROOT\07-Aug-2017\0\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=1610612736\|a6\|0,1\C,1.4567411396,0.0468530919,1.1086255502\C,1.3547894214,1.1533823759,0.0018753907\C,1.5588154856,-1.2920524675,0.3630791327\C,1.4025100157,0.4150708934,-1.3438516235\H,1.0786228019,-2.1192163569,0.8929813356\H,2.6030701776,-1.5710695189,0.1882090188\H,0.7973026764,0.8854304632,-2.1225974317\H,2.4347410507,0.3449214902,-1.7069548383\C,2.6718526923,0.5289815602,1.966163114\C,2.5256608438,2.1219774156,0.3724030747\C,3.8305843757,1.3751440225,0.1574509997\C,3.9167568699,0.4300719662,1.1019590947\C,2.4316277381,2.0551519516,1.913952177\H,2.7361652084,0.0692345787,2.9540384736\H,2.4558931593,3.1094423857,-0.0875468866\H,4.5096413557,1.5271959167,-0.6743638188\H,4.6781011056,-0.3374646583,1.1867111555\H,3.2167214906,2.628229311,2.4137760847\H,1.448271015,2.349334456,2.298415498\C,0.9061712848,-1.0092791743,-0.994104361\H,-0.1872680324,-0.9908068662,-0.9090882832\H,0.5608907523,0.0587168156,1.7394787772\H,0.4086603854,1.6985656123,0.092504358\C,1.2700527934,-1.9996279471,-2.0681261731\O,2.1811698067,-2.7912567958,-2.0287067867\O,0.4677591266,-1.8848607471,-3.1494807136\H,0.7836402599,-2.5205567744,-3.8100243183\Version=ES64L-G09RevE.01\State=1-A\HF=-577.8229013\RMSD=7.073e-09\RMSF=1.852e-05\Dipole=-0.4896496,0.5290665,0.0587355\Quadrupole=-0.7107424,-2.9843807,3.695123,1.7725344,0.0267327,-0.3566967\PG=C01 [X(C11H14O2)]\@

7b(iii) [product]

1\1\GINC-R266\FOpt\RM062X\6-31+G(d,p)\C12H19N1\ROOT\07-Aug-2017\0\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=1610612736\|a6\|0,1\C,1.6544965883,0.0231642722,1.2632377838\C,1.1661436962,1.020942594,0.1592603105\C,1.8676544003,-1.3196991137,0.5528796677\C,1.1166412161,0.2148534895,-1.1450071088\H,1.6359427647,-2.1705530906,1.1996378555\H,2.9031734045,-1.4240763918,0.2052867356\H,0.3076834604,0.5435941618,-1.8033811769\H,2.0621571124,0.2943909953,-1.6961036104\C,2.8916755121,0.7614077006,1.8735089169\C,2.1876762672,2.1996540308,0.2823184619\C,3.5502833059,1.6791151444,-0.1394609364\C,3.9677485292,0.8260175292,0.8041695865\C,2.3727502055,2.2162528662,1.8167744669\H,3.2061000683,0.3833281634,2.8481556725\H,1.862167587,3.1288267156,-0.1893073443\H,4.0362710863,1.8911877269,-1.0854786404\H,4.8593348328,0.2093085043,0.7749256431\H,3.1144631898,2.9471149319,2.1492287948\H,1.4326828853,2.3592429688,2.3619360614\C,0.9676079986,-1.2484410296,-0.6931175074\H,-0.087161597,-1.4190709626,-0.3807493645\H,0.8951720743,-0.0812421687,2.0462334084\H,0.1687718372,1.4027992137,0.4041619363\N,1.3350

169073,-2.2114802164,-1.726009093\C,1.2489152241,-3.5774386875,-1.2336
631658\H,1.5078558348,-4.270058611,-2.0389310743\H,1.9551277086,-3.733
8914156,-0.4159313177\H,0.232711837,-3.830536636,-0.8728400812\C,0.506
4198014,-2.0605863361,-2.91189528\H,-0.5713490807,-2.1878076224,-2.690
1632091\H,0.6536715741,-1.0750135591,-3.357842551\H,0.7936807678,-2.81
13841678,-3.6528458405\Version=ES64L-G09RevE.01\State=1-A\HF=-523.213
2133\RMSD=8.013e-09\RMSF=4.532e-06\Dipole=-0.3028756,-0.0506723,0.0881
979\Quadrupole=-1.1609867,0.4461925,0.7147943,-0.7486383,0.572729,-0.7
692876\PG=C01 [X(C12H19N1)]\@

7b(iv) [product]

1\1\GINC-R343\FOpt\RM062X\6-31+G(d,p)\C12H20N1(1+)\ROOT\07-Aug-2017\0\
\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk
=1610612736\A3\1,1\C,1.3818362155,0.1412624173,1.1444570998\C,1.2588
43772,1.2243925151,0.0191565947\C,1.4190031883,-1.221403732,0.43431526
01\C,1.2277325025,0.4630798076,-1.3157400653\H,0.9141129595,-2.0057597
759,1.0028141766\H,2.4614643351,-1.5300212466,0.2688885292\H,0.5798947
32,0.938262583,-2.0558935264\H,2.2425340332,0.3982648269,-1.7344645388
\C,2.657308944,0.5977601961,1.9267963764\C,2.4799327547,2.1599065736,0
.3038219974\C,3.7495894651,1.3677770586,0.0428780441\C,3.8547722987,0.
4414836111,1.0052560299\C,2.4574791995,2.1288539246,1.8493675274\H,2.7
529843806,0.1574591278,2.919808709\H,2.4146688518,3.1370451316,-0.1757
949637\H,4.4169281755,1.5133627393,-0.7998754607\H,4.6247233007,-0.316
6099901,1.1013817192\H,3.2838406846,2.68551045,2.2948493407\H,1.507018
6341,2.4654015697,2.2771801609\C,0.760320536,-0.9438028296,-0.92265783
45\H,-0.3328777409,-0.9983570607,-0.8556784243\H,0.5203710753,0.184298
7558,1.8171603887\H,0.3368096838,1.8008559863,0.1376780313\N,1.1404586
609,-1.9821522434,-1.9638060849\H,2.1637761855,-1.9446747535,-2.039282
0638\C,0.766103511,-3.3680984647,-1.5443550988\H,1.0527546812,-4.06537
46389,-2.3313311467\H,1.2810661335,-3.6155219202,-0.618243113\H,-0.314
2698231,-3.3962366438,-1.3945088679\C,0.5735132967,-1.6666282274,-3.31
13805123\H,-0.5134096573,-1.6338395383,-3.222132715\H,0.9529041302,-0.
7028625684,-3.6450240719\H,0.8678338997,-2.4487056407,-4.0109734973\Ver
ersion=ES64L-G09RevE.01\State=1-A\HF=-523.5985718\RMSD=4.226e-09\RMSF=
6.863e-06\Dipole=-1.1467288,-2.5132345,-2.2939497\Quadrupole=-7.777016
1,4.7793288,2.9976874,4.3931395,4.3416273,10.6106429\PG=C01 [X(C12H20N
1)]\@

8b(ii) [product]

1\1\GINC-R868\FOpt\RM062X\6-31+G(d,p)\C12H15O2(1-)\ROOT\07-Aug-2017\0\
\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk
=1610612736\A5\1,1\C,1.4462268856,0.0246718419,1.1641841547\C,1.318
1791336,1.0594356868,-0.0055330555\C,1.6533990281,-1.4025207411,0.6657
920899\C,0.568227988,-1.8083966305,-0.3465525469\C,0.4156628798,-0.765
7572922,-1.4782957531\C,1.4183053369,0.3913124588,-1.3742675254\H,1.63
86565919,-2.1188197609,1.4932849141\H,2.6378712851,-1.4910270527,0.186
9084877\H,-0.3744344708,-1.8896184486,0.2121388057\H,-0.5995882217,-0.
3427131313,-1.4668970322\H,1.2387048143,1.1302956489,-2.1677716949\H,2
.4327598357,0.0033807432,-1.5269663248\C,2.5979017241,0.6367466304,2.0
325599825\C,2.4143167393,2.1199795369,0.3483925367\C,3.7641547119,1.43
76059564,0.2097467111\C,3.8721035536,0.5540294327,1.210834333\C,2.2823
260916,2.1403505509,1.8860535378\H,2.6541710486,0.2308656187,3.0454727
705\H,2.3017075778,3.0722220208,-0.1771016112\H,4.4400016598,1.5524026
603,-0.6310541109\H,4.6514132304,-0.1890112651,1.3409912594\H,3.023238
5566,2.7843803842,2.3707189157\H,1.2725990823,2.4003886362,2.225922481
1\H,0.5487557745,-1.2950196637,-2.4266105677\H,0.5275005804,0.04593765
75,1.767085397\H,0.3400574844,1.5579518884,0.0569842911\C,0.8970908416
,-3.2613661404,-0.8470988572\O,1.2121808448,-3.3941817887,-2.052721451
7\O,0.8335264118,-4.1342804374,0.0513678632\Version=ES64L-G09RevE.01\
State=1-A\HF=-616.5624558\RMSD=9.237e-09\RMSF=1.478e-06\Dipole=0.93981
24,5.2988178,1.7571968\Quadrupole=16.3028091,-24.8460622,8.543253,-9.9
400557,-2.9169123,-12.5332605\PG=C01 [X(C12H15O2)]\@

8b(i) [product]

1\1\GINC-R2430\FOpt\RM062X\6-31+G(d,p)\C12H16O2\ROOT\07-Aug-2017\0\#M
062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=16
10612736\A5\0,1\C,1.4136891553,0.019119532,1.1492934153\C,1.30937252

68,1.0656564913,-0.0113217794\C,1.5992676508,-1.4072116459,0.640984402
8\C,0.486826586,-1.765454071,-0.3733206764\C,0.3467322204,-0.711837748
2,-1.4987715389\C,1.3831758964,0.411812776,-1.3880146962\H,1.580144032
1,-2.1198590892,1.471920369\H,2.5753630642,-1.5035560313,0.1506342668\
H,-0.4500191866,-1.8514637958,0.1899641618\H,-0.6558186402,-0.27178247
93,-1.4501558031\H,1.2042781541,1.1564447011,-2.1720503214\H,2.3870630
007,0.0063996926,-1.560879393\C,2.589283113,0.5826581855,2.0154863631\
C,2.4418586434,2.0839552878,0.3430210103\C,3.7693403501,1.3608731665,0
.1917301851\C,3.8581609263,0.469341897,1.1869698443\C,2.3159468392,2.0
955405586,1.8812394588\H,2.6352075996,0.1685849386,3.0248125217\H,2.35
47881361,3.0416389965,-0.1741919874\H,4.4599233014,1.4863487458,-0.635
027874\H,4.6349501331,-0.2739248253,1.3300976752\H,3.0791832734,2.7087
995816,2.3666131441\H,1.3186925546,2.3868484434,2.2303176436\H,0.43536
01022,-1.2083305614,-2.468397173\H,0.4989148492,0.0497479686,1.7556556
523\H,0.3483455055,1.5917491283,0.0632078975\C,0.7826525871,-3.1438237
851,-0.9213604063\O,1.186955308,-3.4073504321,-2.0282773888\O,0.580772
0589,-4.102875491,0.0092335508\H,0.826257259,-4.9495421359,-0.39410952
46\Version=ES64L-G09RevE.01\State=1-A\HF=-617.1216791\RMSD=6.473e-09\
RMSF=2.785e-06\Dipole=-0.215324,0.2267266,0.5984347\Quadrupole=0.87241
6,3.119112,-3.991528,-1.0547393,-0.2898661,-4.1734983\PG=C01 [X(C12H16
O2)]\@

8b(iii) [product]

1\1\GINC-R462\FOpt\RM062X\6-31+G(d,p)\C13H21N1\ROOT\07-Aug-2017\0\#M0
62X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=161
0612736\|a5\0,1\C,1.6637787052,-0.0173867601,1.1216172128\C,1.1735792
149,1.0902571019,0.127384289\C,1.9085775318,-1.3566843778,0.4303577508
\C,0.6495295946,-1.8048082407,-0.3373099222\C,0.1461109217,-0.69231707
,-1.2996315297\C,1.0265863416,0.5616620864,-1.2972729324\H,2.189156991
7,-2.1162575128,1.1707262639\H,2.7521969337,-1.258338923,-0.2626497078
\H,-0.1338124595,-1.9823803667,0.4115392442\H,-0.8719408838,-0.4060987
763,-1.010161513\H,0.5880232789,1.3304287067,-1.9444455523\H,2.0153262
833,0.3268547267,-1.711232629\C,2.9161376176,0.6484904122,1.7830962311
\C,2.2145025705,2.2360373382,0.3482987072\C,3.5589871883,1.7332922758,
-0.1493793638\C,3.9769797209,0.7900439559,0.7044082808\C,2.4279175504,
2.1097822672,1.8716967303\H,3.2357335711,0.1692170957,2.7108517255\H,1
.8936332255,3.2073020799,-0.0341411637\H,4.0298502369,2.0240300239,-1.
0822047901\H,4.8547127177,0.1608919583,0.6033622482\H,3.1925533274,2.7
91477063,2.2527612\H,1.5018126466,2.220862431,2.4472672611\H,0.0640080
815,-1.1090054954,-2.3079047519\H,0.9076403928,-0.1655853934,1.9041196
056\H,0.1921598168,1.4599739496,0.4531174915\N,0.7842309547,-3.0798902
94,-1.0551864097\C,0.8267729281,-4.2327773984,-0.1748781634\H,-0.02900
1071,-4.2103637521,0.506091091\H,0.760605116,-5.1462280696,-0.77438494
83\H,1.7513346226,-4.294944811,0.4279634879\C,1.8908073041,-3.11564151
94,-1.9965893288\H,1.7753950633,-3.9817278314,-2.6556968298\H,1.891201
2249,-2.2162362624,-2.6192084797\H,2.877621739,-3.1934376181,-1.506244
8054\Version=ES64L-G09RevE.01\State=1-A\HF=-562.509117\RMSD=4.847e-09\
RMSF=1.853e-06\Dipole=0.0987856,0.0408115,0.1620535\Quadrupole=-1.298
9524,0.4167002,0.8822522,-2.726852,-2.3105949,-1.7006074\PG=C01 [X(C13
H21N1)]\@

8b(iv) [product]

1\1\GINC-R931\FOpt\RM062X\6-31+G(d,p)\C13H22N1(1+)\ROOT\07-Aug-2017\0\
\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk
=1610612736\|a1\1,1\C,1.4331683001,0.0608824969,1.1917285503\C,1.2833
905382,1.0771903175,0.0087519598\C,1.6533355641,-1.3769193383,0.709898
7313\C,0.52317377,-1.7720047396,-0.2379513039\C,0.2893232117,-0.745764
3946,-1.3746035582\C,1.3151028277,0.3930062106,-1.3562146671\H,1.69989
83218,-2.0522218338,1.5712378006\H,2.6170713512,-1.4215574643,0.191749
5475\H,-0.3992608364,-1.9036165721,0.3374361955\H,-0.7114474597,-0.320
1578099,-1.2499570108\H,1.0769591563,1.107673946,-2.1496985155\H,2.321
7136294,0.0095556637,-1.5658792256\C,2.6275574394,0.6575490408,2.00992
9417\C,2.4190706186,2.1095234978,0.2990757088\C,3.7495411797,1.3940866
073,0.1320821676\C,3.8765052448,0.5345617791,1.1515035626\C,2.33187695
87,2.1627488806,1.8394240612\H,2.701469528,0.2736614199,3.0288146027\H
,2.3075612996,3.0503710632,-0.2416277581\H,4.4330725514,1.5294138471,-
0.6989310744\H,4.6854790219,-0.1686767475,1.3180749137\H,3.1020329595,

2.7942455979,2.2858141058\H,1.3438487621,2.457991043,2.2090429891\H,0.2800030048,-1.2426569539,-2.3537707065\H,0.5360743204,0.0838999381,1.822502679\H,0.3219039885,1.5970248737,0.1014977431\N,0.7563656608,-3.1616889804,-0.8462081349\H,0.0014107169,-3.282022992,-1.5286340969\C,0.6192877659,-4.2661851875,0.1518200632\H,-0.3437079114,-4.1738413556,0.6537430245\H,0.6824487386,-5.2213332232,-0.3701499797\H,1.4299670339,-4.1867921926,0.8746180121\C,2.0441552281,-3.2855931492,-1.599152073\H,2.008724787,-4.1952243577,-2.1988381438\H,2.1731610192,-2.4156041206,-2.2423583607\H,2.8618917093,-3.3477448104,-0.8830412263\Version=ES64L-G09RevE.01\State=1-A\HF=-562.8950451\RMSD=9.567e-09\RMSF=2.602e-06\Dipole=-1.3770747,-3.5797029,-1.2835257\Quadrupole=-7.9068549,14.4910257,-6.5841708,6.6066557,1.808234,6.7450452\PG=C01 [X(C13H22N1)]\@

7c(ii) [product]

1\1\GINC-R1246\FOpt\RM062X\6-31+G(d,p)\C11H13O2(1-)\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=1610612736\|a3|\,1\C,1.7712682652,1.0510906471,0.267816906\C,1.0590332154,0.1291754223,1.3148758299\C,1.759896714,0.2671054949,-1.0602420381\C,0.6642528302,-1.1503126867,0.5497418866\H,2.6815137761,0.416299192,-1.6371615767\H,0.9192525884,0.6105973547,-1.6737713264\H,0.773443129,-2.0518337194,1.1660269019\H,-0.385448689,-1.0769955663,0.2433852535\C,3.1780147637,1.280341031,0.9176624493\C,2.156563401,-0.0421946417,2.4193687637\C,2.3144745648,1.329429303,3.0567761472\C,2.9238574841,2.1184524526,2.1608591831\C,3.4456762303,-0.089360494,1.5740654871\H,3.9322996049,1.6583734118,0.2229570757\H,1.9744472928,-0.8765760458,3.1013606452\H,1.8795664196,1.6312730843,4.0047126886\H,3.0833346286,3.1898565008,2.2349961339\H,4.3492058093,-0.0852493813,2.1922719\H,3.4772236329,-0.9178736144,0.8658488132\C,1.4964306886,-1.2173446449,-0.7446566185\H,1.2679307004,2.0169480286,0.1527335894\H,0.1770751344,0.6048531461,1.7568747585\H,2.4296236705,-1.767094475,-0.593624375\C,0.730648814,-1.940769643,-1.9027448082\O,1.3023323119,-2.9410906287,-2.3946980399\O,-0.3758529809,-1.4314485277,-2.2071486299\Version=ES64L-G09RevE.01\State=1-A\HF=-577.2637413\RMSD=3.946e-09\RMSF=4.872e-06\Dipole=1.9306282,3.1638779,4.0992725\Quadrupole=7.7016653,0.7551431,-8.4568084,-6.6601089,-13.8459553,-20.9785966\PG=C01 [X(C11H13O2)]\@

7c(i) [product]

1\1\GINC-R334\FOpt\RM062X\6-31+G(d,p)\C11H14O2\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=1610612736\|a4|\,1\C,1.7229689094,1.0361548207,0.2864746583\C,1.0699211233,0.0739029411,1.336644536\C,1.7074057011,0.2908838154,-1.0619213049\C,0.7092911459,-1.2204224638,0.5804037886\H,2.6154376633,0.4547735293,-1.6503376407\H,0.8623592451,0.6493227812,-1.6611394506\H,0.9168502509,-2.1186289424,1.1719525188\H,-0.3585876049,-1.2319727084,0.3417555605\C,3.1378791076,1.3009378012,0.8994726089\C,2.1949899512,-0.0658630947,2.4142081867\C,2.3191702344,1.307499577,3.0562539503\C,2.8819196059,2.1215166143,2.1547692184\C,3.4663271558,-0.0622521879,1.541816839\H,3.860590075,1.7113892666,0.1910934009\H,2.0546757082,-0.907938344,3.0952249661\H,1.9117909997,1.5804424281,4.0235254411\H,3.025813682,3.1932897933,2.2364354642\H,4.3807136371,-0.029680019,2.1390532744\H,3.5268185228,-0.8914011732,0.8333517833\C,1.4930098949,-1.210931345,-0.7388123189\H,1.1827903179,1.9818586201,0.1949398889\H,0.1755678911,0.5031648634,1.7951353893\H,2.4606431144,-1.7108269426,-0.6464265112\C,0.7667032688,-1.8906126063,-1.8728755934\O,-0.4073368127,-2.1704625911,-1.9095876672\O,1.5909273331,-2.126944928,-2.9166684833\H,1.0561708787,-2.5226085053,-3.6221695033\Version=ES64L-G09RevE.01\State=1-A\HF=-577.8218346\RMSD=5.197e-09\RMSF=5.163e-06\Dipole=0.5072872,0.2604418,-0.00523\Quadrupole=-5.2330293,1.2518622,3.9811671,-2.6576711,-2.4794253,0.058401\PG=C01 [X(C11H14O2)]\@

7c(iii) [product]

1\1\GINC-R817\FOpt\RM062X\6-31+G(d,p)\C12H19N1\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=1610612736\|a1|\,1\C,1.7188549602,0.9960100125,0.2655189566\C,1.0847201344,0.0510800938,1.341334087\C,1.7917961774,0.1790926361,-1.0376786754\C,0.808659184,-1.2873381478,0.6316944292\H,2.7163116108,0.3776089366,-1.5916008148\H,0.9511146582,0.4499623998,-1.6878500668\H,1.0259681522,

-2.1441230751,1.2795163848\H,-0.2505127009,-1.3429486432,0.3526273904\C,3.0939638128,1.3714841922,0.9101270189\C,2.1837470539,0.0158619676,2.4540894306\C,2.2104312073,1.4190288279,3.0406962679\C,2.7526771481,2.2266246797,2.1209118625\C,3.4786982927,0.056559069,1.6178254029\H,3.8145437574,1.7935418253,0.2061802277\H,2.0698677486,-0.8049043954,3.1656253122\H,1.7568025005,1.7079673957,3.98251778\H,2.8308528665,3.3076467594,2.1605961878\H,4.3716676998,0.1640237786,2.2385998874\H,3.6029719045,-0.7941774658,0.9441837893\C,1.6261864061,-1.3089509572,-0.6741331249\H,2.6188854933,-1.7658252899,-0.4909035559\H,1.1309008947,1.9040951538,0.1088045262\H,0.1583591901,0.4550699841,1.7578840842\N,0.9606334316,-2.0689953561,-1.7337476417\C,1.7258365556,-2.0209835278,-2.9706019726\H,1.2119008458,-2.605369162,-3.7385012139\H,1.8107765194,-0.9930606016,-3.3289034079\H,2.7464354636,-2.4330749649,-2.8467374301\C,0.7651043515,-3.4556776978,-1.3380864617\H,0.1214788678,-3.5159065511,-0.4581242401\H,0.2777950872,-4.0001202012,-2.1513622904\H,1.722050725,-3.962871675,-1.1061521293\Version=ES64L-G09RevE.01\State=1-A\HF=-523.2125091\RMSD=7.573e-09\RMSF=8.300e-06\Dipole=0.0896695,-0.1196447,-0.0525064\Quadrupole=-2.1854255,1.7515124,0.433913,0.0878418,-2.4548209,-0.2668063\PG=C01 [X(C12H19N1)]\@

7c(iv) [product]

1\1\GINC-R1117\FOpt\RM062X\6-31+G(d,p)\C12H20N1(1+)\ROOT\07-Aug-2017\0\#\M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=1610612736\A1\1,C,1.7104814553,1.006901244,0.2694370462\C,1.0760446406,0.0609257031,1.3463022282\C,1.7792902967,0.195248794,-1.0409895905\C,0.790748924,-1.2800260267,0.6382656359\H,2.6969901784,0.3925446992,-1.603331405\H,0.9325362806,0.4784738788,-1.6827744085\H,0.9996992969,-2.1408269464,1.2806794185\H,-0.2739394995,-1.3225811483,0.3667661666\C,3.0907889734,1.3711979998,0.9063517527\C,2.1801071687,0.0140069252,2.4519059808\C,2.2108876506,1.4177100097,3.0390254099\C,2.7525018409,2.2246538671,2.1201228682\C,3.4728341217,0.0548210312,1.6124782115\H,3.8084591021,1.7956242458,0.2018537166\H,2.0632786874,-0.8052459466,3.1637217051\H,1.7757537595,1.6997065465,3.9905982244\H,2.8517071163,3.3028463036,2.1650069798\H,4.3659036173,0.1595601831,2.230651776\H,3.6107631708,-0.8003705113,0.9428273918\C,1.6342676842,-1.2808502468,-0.6445508275\H,2.6032825061,-1.7666061854,-0.5008678233\H,1.1243163181,1.9131365867,0.1070928007\H,0.1486949115,0.4585723969,1.7623636522\N,0.9810854169,-2.0985088177,-1.7473361521\H,0.061080536,-1.6764358605,-1.9180277749\C,1.7551633393,-2.0360920763,-3.0260569801\H,1.244109518,-2.6364961727,-3.7784598288\H,1.8259568212,-1.0012528129,-3.3554167465\H,2.750993133,-2.4401226186,-2.837907937\C,0.7608485522,-3.5201420419,-1.336656317\H,0.1207295962,-3.5470557328,-0.4569337576\H,0.2913750151,-4.0575257765,-2.1604185136\H,1.7328198705,-3.9600414932,-1.1084529026\Version=ES64L-G09RevE.01\State=1-A\HF=-523.5955127\RMSD=6.486e-09\RMSF=5.327e-06\Dipole=-1.1691732,-2.4250914,-2.8190494\Quadrupole=-8.8786806,3.1729623,5.7057182,5.3055733,3.6354677,12.1826252\PG=C01 [X(C12H20N1)]\@

8c(ii) [product]

1\1\GINC-R907\FOpt\RM062X\6-31+G(d,p)\C12H15O2(1-)\ROOT\07-Aug-2017\0\#\M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=1610612736\A4\1,C,1.6093040236,0.9467704136,0.3375849011\C,0.9502687383,0.0666540797,1.4522888745\C,1.5160915142,0.3093049601,-1.0566791501\C,1.9171108888,-1.1722913196,-1.1606525198\C,1.2762604482,-2.030891776,-0.0487736141\C,0.3620695336,-1.2378625448,0.8943912934\H,2.1112555106,0.8784053117,-1.7782678778\H,0.4711685611,0.3987979738,-1.3877990257\H,3.0114249824,-1.2296633126,-1.1084434407\H,2.0482429892,-2.5458468072,0.538641694\H,0.0361503706,-1.8729118104,1.7304074027\H,-0.5482620384,-0.9750767755,0.3394464733\C,3.0582520296,1.1726590083,0.8950428782\C,2.1130951245,-0.0955152903,2.4923702207\C,2.3143041938,1.294811417,3.077505286\C,2.8770908024,2.0508639488,2.1237812147\C,3.3584757198,-0.1719269201,1.5863340964\H,3.7720597403,1.5199069307,0.1442493524\H,1.9617003362,-0.9078832197,3.2089123938\H,1.9345882146,1.6290659608,4.0382781563\H,3.0470384965,3.122767232,2.1558557154\H,4.2880809615,-0.1388689588,2.1636400425\H,3.3690415293,-1.0222617737,0.9089773983\H,0.6820005943,-2.8033157543,-0.5470340234\H,1.1116751794,1.9231454989,0.2849222925\H,0.1340405523,0.6149773431,1.9387867255\C,1.5522106214,-

1.6382424627,-2.6181085448\O,0.592393881,-2.4347524767,-2.7392265783\O
.2.259396501,-1.112899876,-3.510185637\Version=ES64L-G09RevE.01\State
=1-A\HF=-616.5578951\RMSD=4.014e-09\RMSF=5.308e-06\Dipole=0.5373964,2.
2495369,5.0589628\Quadrupole=13.9593286,9.1131279,-23.0724566,-5.59743
13,-4.7152702,-17.154239\PG=C01 [X(C12H15O2)]\@

8c(i) [product]

1\1\GINC-R1307\FOpt\RM062X\6-31+G(d,p)\C12H16O2\ROOT\07-Aug-2017\0\#M
062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=16
10612736\A3\0,1\C,1.5633917139,0.9419316558,0.3400557429\C,0.9453170
094,0.0352856245,1.4556578547\C,1.4513202468,0.328468779,-1.0615970616
\C,1.9116559146,-1.1449785899,-1.1612615949\C,1.2954022252,-2.04260331
29,-0.0636710523\C,0.3785367109,-1.2778316024,0.8988340664\H,2.0170177
329,0.9317893639,-1.7791603301\H,0.398397185,0.3793386418,-1.368928711
2\H,3.0057626624,-1.1565939525,-1.1099074185\H,2.0953110427,-2.5362368
698,0.4964242589\H,0.0978059083,-1.9359381623,1.7293272752\H,-0.554709
0714,-1.0418803385,0.3720272464\C,3.0166515694,1.1965631056,0.86852983
39\C,2.126305786,-0.0985928943,2.4768762539\C,2.2996641341,1.296798533
2,3.0603458144\C,2.8307464396,2.0680704971,2.1030529554\C,3.3635992202
,-0.1389000817,1.5574568509\H,3.7108482934,1.5691615525,0.1113835303\H
,2.0060754107,-0.9131133401,3.1950991988\H,1.9401814733,1.6127789063,4
.0336106697\H,2.9913060318,3.1401477557,2.1365173455\H,4.296601594,-0.
0759632663,2.1228926509\H,3.4041461724,-0.9994070424,0.8918576223\H,0.
7151206088,-2.8363341242,-0.5415717962\H,1.0400992099,1.9027028157,0.2
974678506\H,0.1199585998,0.5560172806,1.9518726519\C,1.5621953115,-1.6
327495857,-2.5508831249\O,0.6688567539,-2.3897434698,-2.8458220424\O,2
.362463375,-1.0772570871,-3.4870920164\H,2.0593177354,-1.3974907918,-4
.3504765245\Version=ES64L-G09RevE.01\State=1-A\HF=-617.1152834\RMSD=7
.611e-09\RMSF=8.400e-06\Dipole=0.2811485,0.449479,0.1424584\Quadrupole
=-2.0852216,-1.4341696,3.5193912,-3.1608188,-3.6911404,-2.9297204\PG=C
01 [X(C12H16O2)]\@

8c(iii) [product]

1\1\GINC-R715\FOpt\RM062X\6-31+G(d,p)\C13H21N1\ROOT\07-Aug-2017\0\#M0
62X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=161
0612736\A6\0,1\C,1.7961682584,0.8279411762,0.2759606401\C,0.87573256
49,0.2989712969,1.4219941609\C,1.6383178707,0.0547800751,-1.0423784651
\C,1.7183700292,-1.4721227275,-0.9260628197\C,0.7920367132,-1.99900122
24,0.2060009295\C,0.0377933317,-0.9008134014,0.9682376191\H,2.40315351
65,0.4174660014,-1.7368264103\H,0.6643973354,0.308881896,-1.4835290126
\H,2.7713273656,-1.7305953076,-0.6917312127\H,1.3588085805,-2.62215674
17,0.9064097777\H,-0.47089639,-1.3449465199,1.8322867927\H,-0.75608458
41,-0.5182115204,0.314495346\C,3.2192186156,0.7846417363,0.93454492\C,
1.8902237145,0.0377783263,2.5867050524\C,2.3868556273,1.4184455538,2.9
921916956\C,3.1801366264,1.8626615529,2.0088553246\C,3.137287065,-0.46
58380673,1.8337024474\H,4.0457511988,0.8393672815,0.2217653718\H,1.497
7064074,-0.5916610873,3.3890331112\H,2.0495621889,1.9703108387,3.86292
37581\H,3.6197090284,2.8498202436,1.9150817305\H,4.0060328176,-0.55375
43816,2.4910799767\H,2.993052793,-1.402339097,1.2979803567\H,0.0405257
369,-2.649975945,-0.2502037517\H,1.5579942044,1.8722330283,0.049480428
3\H,0.1775399508,1.0793548293,1.7422340109\N,1.3666124183,-2.132891116
1,-2.1958924023\C,2.035071856,-1.5514214062,-3.351124618\H,1.80348375,
-2.1558620263,-4.2319642321\H,1.6800318122,-0.5379118907,-3.5421511518
\H,3.1363677723,-1.5258592252,-3.2340586956\C,1.7002351251,-3.54990257
73,-2.1319062492\H,1.2039762437,-4.0303379418,-1.286776764\H,1.3664314
667,-4.0474048652,-3.0463333571\H,2.7904539887,-3.7117837682,-2.025030
3078\Version=ES64L-G09RevE.01\State=1-A\HF=-562.502525\RMSD=6.673e-09
\RMSF=2.297e-06\Dipole=0.0797934,-0.0237973,-0.0656097\Quadrupole=-1.9
96893,1.5743692,0.4225238,-0.355009,-2.8892296,-0.389933\PG=C01 [X(C13
H21N1)]\@

8c(iv) [product]

1\1\GINC-R494\FOpt\RM062X\6-31+G(d,p)\C13H22N1(1+)\ROOT\07-Aug-2017\0\
\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk
=1610612736\A6\1,1\C,1.8205585618,0.8571198124,0.2905141716\C,0.8844
206153,0.3174406475,1.4193275955\C,1.6496317757,0.1204961536,-1.051455
7561\C,1.720489464,-1.3988066112,-0.9180082589\C,0.7466833579,-1.95043

29568,0.153809684\C,0.0148370054,-0.8497570557,0.9389855513\H,2.420855
5921,0.4829792932,-1.7373654343\H,0.6740902825,0.3980917103,-1.4775954
652\H,2.7528604626,-1.699860105,-0.7113803093\H,1.2882853003,-2.612321
0913,0.8348411316\H,-0.4941255025,-1.3130757225,1.7898709711\H,-0.7787
071613,-0.4388050969,0.3028032415\C,3.2416265096,0.7619040714,0.945459
7233\C,1.8902856484,0.0092545485,2.5792567543\C,2.416055183,1.37103681
06,3.0130182574\C,3.2219919437,1.8182948321,2.0433061854\C,3.130856121
9,-0.5035614146,1.8219667962\H,4.0728350124,0.8205462354,0.2381079805\
H,1.4826595774,-0.6255156703,3.3684884149\H,2.0991117264,1.9026515065,
3.9027055008\H,3.6979562884,2.7895282774,1.9747985863\H,3.9945819442,-
0.6197889619,2.4790284924\H,2.9770699818,-1.4396975129,1.2822578307\H,
-0.0206884366,-2.5763956334,-0.3206062457\H,1.6034204624,1.9069714088,
0.0776279163\H,0.1995689918,1.1022598242,1.7513424739\N,1.4222632616,-
2.0841872655,-2.2576786279\H,0.4134773653,-1.9849828081,-2.4162428001\
C,2.1248142878,-1.46987302,-3.4273416434\H,1.9505333675,-2.0953235879,
-4.3027172215\H,1.740294932,-0.4681744179,-3.6040607825\H,3.1920590057
,-1.4320699464,-3.2029404973\C,1.7369884684,-3.5472970606,-2.195778931
5\H,1.2541556367,-3.9917500288,-1.3280604283\H,1.3836471966,-4.0259159
69,-3.1088568738\H,2.8199077698,-3.650956195,-2.1146769835\Version=ES
64L-G09RevE.01\State=1-A\HF=-562.8870491\RMSD=8.691e-09\RMSF=4.653e-06
\Dipole=-0.6093642,-2.1430758,-3.3389268\Quadrupole=-10.6348659,-0.039
1858,10.6740517,2.3730401,0.4284045,12.8574992\PG=C01 [X(C13H22N1)]\@

7d(ii) [product]

11\GINC-R2400\FOpt\RM062X\6-31+G(d,p)\C11H13O2(1-)\ROOT\07-Aug-2017\O
\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdis
k=1610612736\|a1|-1,1\C,1.3853529796,1.1369433388,0.199222386\C,0.76
78157541,0.1532860018,1.254113039\C,1.4461460106,0.3413269457,-1.11726
85011\C,0.5056063199,-1.156695002,0.4892437008\C,0.3834605548,2.334401
2028,0.2207716531\C,-0.5031745718,0.9220603584,1.7354655792\C,0.002045
0117,2.1429022433,2.4907314034\C,0.5293587654,2.9830087823,1.589763335
4\C,-0.9532594241,1.5880946879,0.417734786\H,2.3093636167,0.6181779136
,-1.7323086218\H,0.5427139995,0.505311862,-1.717915666\H,0.6391618719,
-2.042024925,1.1204473406\H,-0.5167337008,-1.1820215609,0.0916896481\H
,0.0405171067,2.2366106029,3.5717662789\H,1.0817567852,3.8954498108,1.
7927485281\H,-1.1748306674,0.8727229071,-0.3789863411\H,-1.7980035985,
2.2695876541,0.5586987885\H,0.4596594982,2.9986300354,-0.6438347175\H,
-1.2359442756,0.2976639134,2.2528899152\C,1.4608267835,-1.142067208,-0
.7149154559\H,2.4699099218,-1.4393442788,-0.4013162868\H,2.3851068019,
1.4723603265,0.4976640821\H,1.4502517766,-0.0168119111,2.0946013656\C,
0.9955706534,-2.0858133162,-1.8671314083\O,1.8056812212,-2.9736009097,
-2.2194100801\O,-0.1538791944,-1.8396994751,-2.3117246038\Version=ES6
4L-G09RevE.01\State=1-A\HF=-577.2667948\RMSD=5.910e-09\RMSF=4.976e-06\
Dipole=-0.2479454,0.06083,3.6411303\Quadrupole=12.2660147,-10.188785,-
2.0772297,6.0659453,1.6647808,-23.7288261\PG=C01 [X(C11H13O2)]\@

7d(i) [product]

11\GINC-R805\FOpt\RM062X\6-31+G(d,p)\C11H14O2\ROOT\07-Aug-2017\O\#M0
62X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=161
0612736\|a5|\0,1\C,1.4000275855,1.1037313268,0.2104861735\C,0.71326039
74,0.1390224229,1.2406751304\C,1.4699090348,0.3238240379,-1.1146038296
\C,0.4141367547,-1.1584633298,0.4687703226\C,0.4507336673,2.3407753582
,0.2154034424\C,-0.5366157229,0.9543443716,1.6930274488\C,0.0082081366
,2.142625611,2.4738226035\C,0.5943853435,2.9658015347,1.5963854794\C,-
0.9232398531,1.6571431841,0.3747184914\H,2.3583464716,0.5688432572,-1.
7032639657\H,0.5956503774,0.5277615671,-1.7431414987\H,0.4972733774,-2
.0549254183,1.0884566319\H,-0.6004062718,-1.1327254763,0.051088557\H,0
.0076555049,2.2278450538,3.5549135207\H,1.16870287,3.8587901926,1.8172
910348\H,-1.1720527056,0.9698342641,-0.4396732058\H,-1.7358397957,2.37
53333368,0.5063995192\H,0.5804886034,3.0103590518,-0.6374540399\H,-1.3
071636075,0.3599446513,2.1889108488\C,1.4343467122,-1.1481778109,-0.69
33018948\H,2.4096683766,-1.4703715037,-0.3112653039\H,2.4046342174,1.3
893895792,0.5362185882\H,1.3650534872,-0.0736533181,2.0932383803\C,1.0
178848008,-2.0905971992,-1.7914457539\O,0.3440751625,-1.8023786312,-2.
7517057446\O,1.4422230901,-3.3523341374,-1.5663550546\H,1.0960369855,-
3.9046749764,-2.2844178815\Version=ES64L-G09RevE.01\State=1-A\HF=-577
.8246056\RMSD=5.627e-09\RMSF=6.457e-06\Dipole=0.3318078,-0.141458,0.55

4326\Quadrupole=-0.1887059,3.5017326,-3.3130267,1.0902699,-1.9077034,0.3041906\PG=C01 [X(C11H14O2)]\@

7d(iii) [product]

1\1\GINC-R939\FOpt\RM062X\6-31+G(d,p)\C12H19N1\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=1610612736\|a2\|0,1\|C,1.2732475049,0.9980582437,0.1501337852\|C,0.5230541481,0.0400281326,1.1372169389\|C,1.3490991048,0.2297351544,-1.1824219585\|C,0.204483975,-1.2124674214,0.3048409789\|C,0.3738649462,2.2716833943,0.1579959583\|C,-0.7042858998,0.8940196022,1.5800711972\|C,-0.1296164894,2.0409730407,2.4009258846\|C,0.5106002446,2.8587254923,1.5565998542\|C,-1.0320928291,1.6465090568,0.2728199408\|H,2.2335919606,0.4965818416,-1.7648275165\|H,0.4752223579,0.4483430847,-1.8087681708\|H,0.1210486629,-2.123597812,0.9006074879\|H,-0.754734137,-1.0904322249,-0.2123529277\|H,-0.1483113362,2.1000383318,3.4836761659\|H,1.1196448943,3.7189002093,1.8122406745\|H,-1.2950363434,0.991661243,-0.5634558032\|H,-1.815516194,2.3964534872,0.4062911464\|H,0.549571367,2.9569329165,-0.6744401385\|H,-1.5117907631,0.3227511308,2.0438621073\|C,1.3017598606,-1.2537960214,-0.702910642\|H,1.0125166201,-1.9164654214,-1.6103588543\|H,2.2807694414,1.2284465365,0.5040701376\|H,1.1469979528,-0.2233754002,1.99639519\|N,2.6060566141,-1.6709028181,-0.2352612973\|C,2.5429410644,-2.8975294258,0.5449511471\|H,2.0012023444,-2.7416307036,1.4795310781\|H,2.0645678644,-3.7289513235,-0.0078855949\|H,3.559735442,-3.2043502486,0.8030610496\|C,3.5729829393,-1.8418115079,-1.3099559929\|H,3.2844629801,-2.6564896103,-2.0020619194\|H,3.6768509485,-0.924889182,-1.8917377818\|H,4.5521337538,-2.0812917773,-0.887008703\|Version=ES64L-G09RevE.01\|State=1-A\|HF=-523.211929\|RMSD=5.070e-09\|RMSF=1.796e-06\|Dipole=0.0476936,-0.2934502,-0.1665266\|Quadrupole=-0.4201578,-0.0854543,0.5056122,0.5680108,-0.6152448,-1.0910176\|PG=C01 [X(C12H19N1)]\@

7d(iv) [product]

1\1\GINC-R1900\FOpt\RM062X\6-31+G(d,p)\C12H20N1(+)\ROOT\07-Aug-2017\0\|a2\|0,1\|C,1.2827727574,0.9990526169,0.1677190884\|C,0.5195147656,0.026035803,1.1381603078\|C,1.3685124434,0.2521326267,-1.1810298291\|C,0.1958845523,-1.2170614216,0.2877247\|C,0.3828278983,2.27365001,0.1826597347\|C,-0.7093593295,0.8796932624,1.5796246827\|C,-0.1355782778,2.0142235341,2.4188800673\|C,0.5116916295,2.841043967,1.5905707453\|C,-1.0216608894,1.6441389819,0.2764987825\|H,2.2560348649,0.513999904,-1.7632329184\|H,0.5048740781,0.4855994477,-1.8118151209\|H,0.1060253345,-2.1436745815,0.8575624722\|H,-0.7596336138,-1.0864077902,-0.2314107597\|H,-0.1875351649,2.0713048494,3.4998824188\|H,1.0985375464,3.7130677576,1.854630397\|H,-1.2886656784,1.0054927396,-0.572153907\|H,-1.8027441993,2.3935143638,0.4130414278\|H,0.5724460027,2.9651934325,-0.6400231723\|H,-1.5172902919,0.3012297042,2.0309134612\|C,1.2683951724,-1.2315633726,-0.8024018658\|H,1.057216315,-1.9121744897,-1.6328850041\|H,2.2851069328,1.2539363102,0.5319821176\|H,1.1212710851,-0.2494629778,2.0125667414\|N,2.6281295912,-1.6891310683,-0.256393927\|H,2.9769737069,-0.9171042249,0.323722119\|C,2.5610139,-2.9066634419,0.6098726537\|H,2.052842972,-2.6665661632,1.5411897385\|H,2.0169346835,-3.6824901482,0.068864899\|H,3.577389713,-3.2399023658,0.8188368745\|C,3.6089386092,-1.9122046886,-1.3651573154\|H,3.294229368,-2.7991111298,-1.9167140383\|H,3.6209926946,-1.0477903684,-2.0250403581\|H,4.5985178281,-2.0709360786,-0.9372332132\|Version=ES64L-G09RevE.01\|State=1-A\|HF=-523.5959311\|RMSD=4.931e-09\|RMSF=6.994e-06\|Dipole=2.12349,-2.5284319,-0.9171534\|Quadrupole=0.9619875,4.4479875,-5.4099751,-9.7938439,-4.2603491,3.1956484\|PG=C01 [X(C12H20N1)]\@

8d(ii) [product]

1\1\GINC-R882\FOpt\RM062X\6-31+G(d,p)\C12H15O2(1-)\ROOT\07-Aug-2017\0\|a5\|0,1\|C,1.2302809519,1.0051553118,0.2109134413\|C,0.5990766775,0.1067804793,1.3305276057\|C,1.2579880454,0.3065774363,-1.1497517092\|C,1.9298172976,-1.0752803583,-1.0830639893\|C,1.3676806805,-1.9334975326,0.0716838173\|C,0.191936273,-1.2671735367,0.7945674896\|C,0.3179654012,2.2774455289,0.246320412\|C,-0.5915838709,0.9818160699,1.8448626533\|C,0.0385381385,2.1799781701,2.5352211834\|C,0.58152611,2.9504949902,1.5821378229\|C,-1.0583225599,1.6424941039,0.5321234969\|H,1.7921830934

,0.9150113344,-1.8857799954\H,0.2347442748,0.186393529,-1.5325889991\H
,3.0036530284,-0.9030687906,-0.9300560877\H,2.1547754111,-2.1328595953
,0.8136166506\H,-0.1561933088,-1.8951176588,1.6259950969\H,-0.65267139
87,-1.1737176182,0.0998751141\H,0.1447804456,2.2958659237,3.6094192906
\H,1.2164536906,3.8189349783,1.7275223771\H,-1.3740341438,0.9258591034
,-0.2307378267\H,-1.8429543481,2.388657843,0.6915748388\H,0.4036727887
,2.9056865418,-0.6435913451\H,-1.3378815587,0.425228783,2.4185267655\H
,1.0519457449,-2.8901710903,-0.3548041698\H,2.2592027077,1.2795827082,
0.4757976663\H,1.3181492686,-0.05087229,2.1450588181\C,1.7902561124,-1
.7342462532,-2.5021813773\O,2.4331334417,-1.1445928765,-3.4029704807\O
,1.0385886053,-2.7329682348,-2.5947645605\Version=ES64L-G09RevE.01\St
ate=1-A\HF=-616.5638091\RMSD=6.894e-09\RMSE=5.275e-06\Dipole=-1.351595
8,3.0928086,4.5988056\Quadrupole=13.7115354,-0.1778057,-13.5337297,5.3
961795,11.7778396,-21.2565307\PG=C01 [X(C12H15O2)]\@

8d(ii) [product]

1\1\GINC-R1076\FOpt\RM062X\6-31+G(d,p)\C12H16O2\ROOT\07-Aug-2017\0\#M
062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=16
10612736\|a4\|0,1\C,1.2612304313,0.9605240429,0.2133818923\C,0.5805387
684,0.091103187,1.3263330138\C,1.2878530405,0.2562775914,-1.1435562369
\C,1.9314126784,-1.1447383738,-1.02327919\C,1.2999019701,-1.9900214156
,0.107680791\C,0.1351525642,-1.2722485818,0.7957465595\C,0.387309615,2
.2572918538,0.2116688872\C,-0.591256845,1.0075648799,1.805790018\C,0.0
647477331,2.192948629,2.494962625\C,0.6481651567,2.9360969812,1.546359
0076\C,-1.013235811,1.6685911708,0.4782919494\H,1.8496722231,0.8543100
68,-1.86777536\H,0.2694536248,0.1513679003,-1.5381680398\H,3.001374866
8,-0.9935412171,-0.8382600039\H,2.0672893725,-2.209419465,0.8584969133
\H,-0.238027554,-1.8865921074,1.6225398187\H,-0.6992831482,-1.16029179
43,0.0924405388\H,0.1361019391,2.3260857031,3.568941783\H,1.2910892365
,3.7976345976,1.6896030224\H,-1.3494946267,0.9576508238,-0.2826336027\
H,-1.7728510131,2.4416388073,0.616748939\H,0.5108405866,2.8756541559,-
0.680498632\H,-1.3632014982,0.4813263345,2.3719149191\H,0.9631084685,-
2.9460064364,-0.3011969133\H,2.2936536893,1.2050281904,0.489669756\H,1
.2791590506,-0.0817076421,2.1536406997\C,1.8205084021,-1.8246607124,-2
.369720085\O,1.075990601,-2.7305067801,-2.6584968291\O,2.6459734365,-1
.2633597395,-3.2802181803\H,2.4942320409,-1.7170986514,-4.1234250606\
Version=ES64L-G09RevE.01\State=1-A\HF=-617.1216614\RMSE=4.262e-09\RMSE
=6.881e-06\Dipole=0.3615279,0.4466399,0.1671694\Quadrupole=0.5194461,-
4.6892391,4.1697929,-0.9734711,-1.8231143,-2.9841662\PG=C01 [X(C12H16O
2)]\@

8d(iii) [product]

1\1\GINC-R1232\FOpt\RM062X\6-31+G(d,p)\C13H21N1\ROOT\07-Aug-2017\0\#M
062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=16
10612736\|a2\|0,1\C,1.1492249178,0.9877842882,0.2018952793\C,0.5382035
661,0.0960205877,1.3386595858\C,1.1368432099,0.2839418393,-1.157174343
7\C,1.84289434,-1.0825365946,-1.0744860686\C,1.2583551247,-1.950657367
9,0.0732301383\C,0.1030983552,-1.2750353304,0.8169621148\C,0.246172276
5,2.2636417122,0.2501218232\C,-0.6327163086,0.9807780423,1.875508526\C
,0.0240686027,2.1771759573,2.5448334749\C,0.5474091449,2.9404735488,1.
5773307829\C,-1.1274386606,1.6405187219,0.5725711376\H,1.632453406,0.9
18086421,-1.9021055853\H,0.1027400846,0.1508271782,-1.4975164716\H,2.8
965940733,-0.8800486788,-0.8416156719\H,2.0543642517,-2.1708556835,0.7
941082829\H,-0.2224787947,-1.9030538748,1.6541121611\H,-0.764697686,-1
.1715092403,0.1521704052\H,0.1400226899,2.3040370725,3.6157281502\H,1.
1760944942,3.8157427767,1.6996773087\H,-1.4777056891,0.9265582337,-0.1
791617745\H,-1.8990491636,2.3937392801,0.7496517581\H,0.3156749202,2.8
904156306,-0.6420493751\H,-1.3669285098,0.4327726515,2.4707796514\H,0.
948541819,-2.9170494018,-0.335547289\H,2.1855027264,1.2565402409,0.439
445768\H,1.2756206159,-0.066463674,2.133807475\N,1.8702417409,-1.84281
40321,-2.3314036715\C,0.5581727615,-2.0829612533,-2.9080758611\H,0.641
0635109,-2.8487621002,-3.6854825285\H,-0.1323677647,-2.4524822997,-2.1
443168375\H,0.1124278796,-1.1827159343,-3.3677208292\C,2.7680245819,-1
.2804007363,-3.3233725867\H,3.7598816381,-1.136243998,-2.8853227192\H,
2.8638450529,-1.9798248245,-4.1598361063\H,2.4234967924,-0.3135131583,
-3.7338401035\Version=ES64L-G09RevE.01\State=1-A\HF=-562.5091384\RMSE
=8.929e-09\RMSE=1.454e-05\Dipole=-0.0235055,0.1229814,-0.0685723\Quadr

upole=0.308525,-2.4769928,2.1684677,2.9580756,0.3857471,-1.2798793\PG=C01 [X(C13H21N1)]\@

8d(iv) [product]

1\1\GINC-R1479\FOpt\RM062X\6-31+G(d,p)\C13H22N1(1+)\ROOT\07-Aug-2017\0
\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdis
k=1610612736\|a2\|1,1\C,1.160763115,0.981230836,0.2060717171\C,0.55100
02266,0.0923134333,1.3461130237\C,1.150442571,0.2706902556,-1.15584163
73\C,1.8689524749,-1.0680694222,-1.0182738074\C,1.2787440919,-1.963348
2196,0.0992822188\C,0.118972226,-1.2845590001,0.8357888405\C,0.2425254
479,2.2463921968,0.2292805351\C,-0.6294977991,0.9733363811,1.866928838
7\C,0.0179551123,2.1822086597,2.524033367\C,0.5371513354,2.9391523435,
1.5509406598\C,-1.1256791204,1.614176786,0.5554961978\H,1.6410158541,0
.9086320802,-1.8988521042\H,0.1147082393,0.1205584124,-1.4783545121\H,
2.9287307057,-0.8774264941,-0.8192911084\H,2.0732210006,-2.1877341794,
0.8178767704\H,-0.1910542183,-1.9147717755,1.6742846575\H,-0.753330195
7,-1.1966963222,0.1757071372\H,0.1123116179,2.3296122994,3.5936415261\
H,1.1425278042,3.8313821568,1.6605352118\H,-1.4806024768,0.8926659416,
-0.188952662\H,-1.900841211,2.3638874148,0.7228881747\H,0.3122484093,
2.8658566811,-0.6677291253\H,-1.358871835,0.4265197635,2.4675467274\H,
0.9558258649,-2.9323130856,-0.3037361385\H,2.1942256145,1.2623817505,0
.4371762344\H,1.2859908191,-0.0594924502,2.1442172096\N,1.8925686017,-
1.8478820864,-2.3392302243\H,2.2613231086,-2.7728525354,-2.0965353393\
C,0.5363012022,-2.0626693103,-2.9338616804\H,0.6134131519,-2.823465408
2,-3.7106577921\H,-0.1530275532,-2.3887620782,-2.1552290029\H,0.195681
3333,-1.1240553195,-3.368512021\C,2.8263355098,-1.2595892933,-3.347889
2639\H,3.8192710992,-1.1771757089,-2.9064716011\H,2.855122723,-1.91022
40672,-4.2222573202\H,2.4579211489,-0.2750956361,-3.6328401029\Versio
n=ES64L-G09RevE.01\State=1-A\HF=-562.8935257\RMSE=3.580e-09\RMSEF=4.383
e-06\Dipole=1.5565743,-2.6559359,-3.0050817\Quadrupole=-7.3137607,-0.0
265683,7.3403289,-4.889212,-8.3449406,12.6830503\PG=C01 [X(C13H22N1)]\
\@

3a(ii)[product]

1\1\GINC-R2477\FOpt\RM062X\6-31+G(d,p)\C11H11O4(1-)\ROOT\07-Aug-2017\0
\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdis
k=1610612736\|a1\|1,1\C,1.1632466643,0.1079732015,1.4104415055\C,0.99
97818815,0.0691762546,0.1989373158\C,1.2144131408,-1.3146576413,0.8134
261028\C,0.9886010495,0.1739316697,-1.0551599606\C,-0.0327942772,0.352
7032666,2.3943840927\C,-0.2957663439,1.8792365406,0.424646079\C,-1.467
1945312,0.9467785066,0.5927274452\C,-1.3283435812,0.1403064718,1.64494
55682\H,0.7129550741,-2.0515548464,1.4527322899\H,2.2596686086,-1.6223
940411,0.6976628664\H,0.3225641957,0.5567601179,-1.8391327966\H,2.0004
953014,0.1194817559,-1.471310769\H,-2.2874376325,0.915569787,-0.115398
9126\H,-2.0332102854,-0.6329551174,1.9309115549\H,0.0600956171,-0.2410
584016,3.3033301589\H,-0.4454714337,2.6416801092,-0.340226656\O,-0.109
6087888,2.620684198,1.6655417162\C,0.0352342023,1.8269785796,2.7468722
795\O,0.2228345742,2.2950331214,3.8446203689\C,0.6129819131,-1.2464770
105,-0.6002801406\H,-0.4712033655,-1.3774850239,-0.5751252083\H,2.0790
760116,0.3358469094,1.9663001619\H,1.8139983638,1.8014948423,0.1661700
395\C,1.2070154385,-2.3361740002,-1.5543491772\O,2.4584644447,-2.32639
67164,-1.6501217369\O,0.3728937581,-3.0825525332,-2.1140341875\Versio
n=ES64L-G09RevE.01\State=1-A\HF=-726.4984433\RMSE=9.889e-09\RMSEF=2.456
e-06\Dipole=-1.7156371,3.1824005,2.3846414\Quadrupole=18.7486729,-11.4
824017,-7.2662712,9.3262307,8.7528456,-37.1974566\PG=C01 [X(C11H11O4)]\
\@

3a(i) [product]

1\1\GINC-R3235\FOpt\RM062X\6-31+G(d,p)\C11H12O4\ROOT\07-Aug-2017\0\#M
062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=16
10612736\|a2\|0,1\C,1.2131543978,0.1743534297,1.3896820113\C,0.9693913
682,1.1149945447,0.1734393687\C,1.3640683652,-1.2491557385,0.816628842
\C,0.9901185711,0.2263026361,-1.0835251041\C,0.0161132465,0.3336426654
,2.3825648501\C,-0.3717063271,1.8441675437,0.4182030121\C,-1.481417030
2,0.8392785743,0.6038378725\C,-1.2763111721,0.0417105743,1.6535244983\
H,0.9043929991,-2.0148876267,1.4482475398\H,2.4291394678,-1.4918679117
,0.7288685069\H,0.2611260878,0.5431503072,-1.8373423776\H,1.9756103553

,0.2625943212,-1.5569113004\H,-2.3356199574,0.790837459,-0.0622875696\
H,-1.9497542667,-0.7444169826,1.9783696986\H,0.1604085013,-0.249695393
1,3.2912406499\H,-0.5783319656,2.5910058294,-0.3481435531\O,-0.2048567
909,2.5934631778,1.6471345144\C,-0.0002171467,1.8145242842,2.734271482
9\O,0.1766913958,2.2878065781,3.8246907932\C,0.7348905285,-1.203882413
2,-0.597067964\H,-0.3346689599,-1.4158067294,-0.5208400544\H,2.1198497
003,0.4624320988,1.9287852475\H,1.7381536527,1.890755242,0.1183101291\
C,1.3424048305,-2.2561125064,-1.4901549715\O,2.1368569353,-2.067342582
8,-2.3791036829\O,0.917093307,-3.4922741903,-1.1551196512\H,1.36706790
66,-4.122526191,-1.7390207887\Version=ES64L-G09RevE.01\State=1-A\HF=-
727.0461766\RMSD=6.020e-09\RMSF=8.888e-06\Dipole=-0.4087367,-1.3786044
,-0.9962204\Quadrupole=6.1857493,1.9814438,-8.1671931,1.1587403,4.9722
983,-10.5638615\PG=C01 [X(C11H12O4)]\@

3a(iii) [product]

1\1\GINC-R3403\FOpt\RM062X\6-31+G(d,p)\C12H17N1O2\ROOT\07-Aug-2017\0\
#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=
1610612736\|a3\|1,C,1.0897259636,0.1553811927,1.4173468862\C,0.92698
22602,1.1062210057,0.1974038286\C,1.1511974162,-1.273053363,0.84441415
23\C,0.9230045299,0.213868151,-1.0544422622\C,-0.1071608207,0.40038656
01,2.3941884162\C,-0.3718308995,1.9162706458,0.4138453538\C,-1.5430242
211,0.9824061538,0.589120117\C,-1.4041851742,0.184001522,1.6486308508\
H,0.6227884053,-1.9903842419,1.4813665464\H,2.1962468853,-1.5970972778
,0.7725297338\H,0.2328849248,0.5843220248,-1.8210683528\H,1.9263296723
,0.1899730237,-1.4953470939\H,-2.3851587663,0.9761181741,-0.0937064359
\H,-2.1278752083,-0.5594911826,1.965375126\H,-0.0121938058,-0.18383622
76,3.3088146714\H,-0.5211508464,2.6687491196,-0.3604608537\O,-0.177543
0488,2.663811922,1.6403469164\C,-0.0350914278,1.881475109,2.735126879\
O,0.1576069952,2.3525139793,3.824342032\C,0.5854472496,-1.2133024273,-
0.5865240543\H,-0.5133505629,-1.3423145128,-0.555403669\H,2.0057287911
,0.3848772081,1.968940612\H,1.7408580126,1.8359031846,0.1574886762\N,1
.1686545513,-2.2337462859,-1.4562896099\C,0.888464162,-3.570962922,-0.
9535056259\H,1.3220218413,-4.3109592931,-1.6310574428\H,1.3390195408,-
3.7123990849,0.031060798\H,-0.1979906816,-3.7686278037,-0.873246147\C,
0.6674882232,-2.1100629192,-2.8173989007\H,-0.4347188835,-2.2030598597
,-2.8675783554\H,0.9529180668,-1.1466913401,-3.2450852769\H,1.10580985
54,-2.8960362348,-3.4376795159\Version=ES64L-G09RevE.01\State=1-A\HF=
-672.4372313\RMSD=5.308e-09\RMSF=7.859e-06\Dipole=-0.3118507,-1.404658
,-1.5716592\Quadrupole=5.4283183,-1.8471708,-3.5811475,1.3754238,1.462
5105,-11.096634\PG=C01 [X(C12H17N1O2)]\@

3a(iv) [product]

1\1\GINC-R303\FOpt\RM062X\6-31+G(d,p)\C12H18N1O2(1+)\ROOT\07-Aug-2017\
0\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdi
sk=1610612736\|a6\|1,C,1.2368306582,0.3737206097,1.3191817788\C,0.71
61853977,1.1198012872,0.0547013475\C,1.4889517882,-1.0870659034,0.8909
659164\C,0.6914648446,0.0897098183,-1.0895447231\C,0.1707852378,0.5175
253044,2.4497091396\C,-0.6708997834,1.710604091,0.4056691827\C,-1.6018
401388,0.6123893018,0.8627875532\C,-1.1571121774,-0.0119590114,1.95672
40595\H,1.2156735572,-1.7999049695,1.6741883622\H,2.5587256119,-1.2213
029679,0.6771668976\H,-0.1608730723,0.2329845329,-1.7609506925\H,1.606
274455,0.1931060734,-1.6894300243\H,-2.5432395796,0.4074738729,0.36451
36539\H,-1.6922233714,-0.793412605,2.486653329\H,0.5109509496,0.081340
5478,3.388230366\H,-1.0729607841,2.3192649441,-0.4041017887\O,-0.43741
94359,2.6236941357,1.4951633137\C,0.008482459,2.0254529267,2.629695306
4\O,0.268454896,2.6489645281,3.6164150836\C,0.6843854499,-1.2816435561
,-0.4011216383\H,-0.3336966117,-1.6219002678,-0.1931169682\H,2.1665297
464,0.8187857501,1.6810949233\H,1.3631901863,1.9619220567,-0.201651322
3\N,1.2834518036,-2.3608859685,-1.2839165123\H,2.244751255,-2.07015035
02,-1.4970684711\C,1.3546986339,-3.6821036203,-0.5835400113\H,1.784175
2426,-4.4185466108,-1.2623762467\H,1.9743742404,-3.5866196257,0.306071
8516\H,0.34012238,-3.973362062,-0.3077598767\C,0.5515909964,-2.4944386
947,-2.582866948\H,-0.4853328271,-2.7514616722,-2.3614877328\H,0.59910
04344,-1.550918235,-3.1232579965\H,1.0162115577,-3.2863276602,-3.16992
81126\Version=ES64L-G09RevE.01\State=1-A\HF=-672.8092341\RMSD=4.713e-
09\RMSF=4.727e-06\Dipole=1.1765635,-4.8941827,-3.9691499\Quadrupole=-2
.4602354,3.0914292,-0.6311938,-5.8938664,-3.8441227,3.9339868\PG=C01 [

X(C12H18N1O2)]\@

5a(ii) [product]

1\1\GINC-R172\FOpt\RM062X\6-31+G(d,p)\C12H13O4(1-)\ROOT\07-Aug-2017\0\#\M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=2147483648\#a4\1,1\C,1.2631400896,0.175672495,1.2712166211\C,1.0471199363,1.1786893678,0.1010269283\C,1.4912081114,-1.2622965525,0.7882461551\C,0.4846883506,-1.7792622639,-0.2492698738\C,0.2652312626,-0.7812055439,-1.4016777649\C,1.0973262738,0.5016566246,-1.2758117226\C,0.0568602964,0.3232009247,2.2662985458\C,-0.26764522,1.9441041532,0.384827253\C,-1.4253955175,0.9936429525,0.5311658194\C,-1.2491223797,0.1301571922,1.5319300606\H,1.5073471492,-1.9554228241,1.6350517918\H,2.4956612978,-1.3023485199,0.3434531641\H,-0.4640795133,-1.9662095061,0.2679519544\H,-0.7977382601,-0.5208738852,-1.4765694491\H,0.8046735883,1.2277605818,-2.047801785\H,2.146205499,0.2532341077,-1.4785924727\H,-2.2750123903,1.0092980867,-0.1416904398\H,-1.9439833841,-0.6554347746,1.8072373782\H,0.1785564706,-0.3195074901,3.1376013928\H,-0.4393857818,2.742001383,-0.3390645596\O,-0.0694252857,2.6254184206,1.6580764472\C,0.0968239691,1.7780681151,2.6974311352\O,0.2871309424,2.1945904113,3.8147060977\H,0.5433015567,-1.2959815499,-2.3268023954\H,2.1495652963,0.4824554549,1.8403158486\H,1.8308532452,1.9456807656,0.137594934\C,0.989439012,-3.1980214499,-0.7110695588\O,1.3588128258,-3.3124950431,-1.9016986665\O,0.9878355594,-4.0528796335,0.2050861609\Version=ES64L-G09RevE.01\State=1-A\HF=-765.7924654\RMSD=3.929e-09\RMSF=3.777e-06\Dipole=-1.3058386,4.3321293,0.6123982\Quadrupole=26.2473724,-28.7233646,2.4759922,1.05793094,5.6595497,-27.5579161\PG=C01 [X(C12H13O4)]\@

5a(i) [product]

1\1\GINC-R543\FOpt\RM062X\6-31+G(d,p)\C12H14O4\ROOT\07-Aug-2017\0\#\M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=2147483648\#a4\0,1\C,1.2884606467,0.1998303315,1.251143438\C,1.0277195078,1.207447744,0.0941474839\C,1.5830545877,-1.22001042,0.7530955041\C,0.5732042303,-1.7446991601,-0.2915728863\C,0.330153257,-0.7502596831,-1.4460217509\C,1.1136742451,0.5585471732,-1.2924856562\C,0.0888687772,0.2831341895,2.2557570345\C,-0.318473616,1.9105879915,0.3934583614\C,-1.4346384196,0.9084337274,0.5393760698\C,-1.2192510422,0.0483200307,1.5358876635\H,1.6268620251,-1.9109002093,1.6010317276\H,2.5820040343,-1.2161600244,0.298763234\H,-0.3661195985,-1.9578069175,0.229227196\H,-0.7405747272,-0.5375367453,-1.5095161643\H,0.7833992651,1.2744505778,-2.0545129104\H,2.1713491537,-0.3633598331,-1.5039552569\H,-2.3076803897,0.9176175187,-0.1035061068\H,-1.9023848273,-0.7389529412,1.8373478416\H,0.2446454146,-0.3556668548,3.1247579784\H,-0.5297738668,2.7044183768,-0.3232427473\O,-0.1369497464,2.5846888679,1.6661740153\C,0.0768139041,1.7397802103,2.7008381052\O,0.266330646,2.1440377624,3.8167789177\H,0.618265182,-1.2224265797,-2.388860658\H,2.1713843217,0.523662329,1.8127096806\H,1.7783018943,2.0038481874,0.1406798156\C,1.0843593213,-3.0802105013,-0.7915799959\O,1.5478003442,-3.3111520343,-1.8817556115\O,0.9994097693,-4.0291880845,0.1651722657\H,1.3716957062,-4.8455766958,-0.2024095884\Version=ES64L-G09RevE.01\State=1-A\HF=-766.3401335\RMSD=4.573e-09\RMSF=9.801e-06\Dipole=-0.2039817,-1.0520238,-1.051419\Quadrupole=8.3747056,0.9689701,-9.3436756,1.1931148,3.4818883,-14.9757896\PG=C01 [X(C12H14O4)]\@

5a(iii) [product]

1\1\GINC-R716\FOpt\RM062X\6-31+G(d,p)\C13H19N1O2\ROOT\07-Aug-2017\0\#\M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=2147483648\#a1\0,1\C,1.2347820553,0.1878305297,1.2924752908\C,1.0372066764,1.1849732156,0.1137961567\C,1.5060509068,-1.2465364631,0.8180104285\C,0.5178199944,-1.7803348097,-0.2367156516\C,0.3245716267,-0.7796402445,-1.4028154587\C,1.1395345587,0.5106009676,-1.2602980462\C,0.0082916148,0.3232838244,2.259455521\C,-0.2936318073,1.9350310107,0.3643784642\C,-1.4447774932,0.9712256498,0.4917426972\C,-1.2848898599,0.1190704548,1.505263967\H,1.5273798797,-1.9168835565,1.6858801238\H,2.5178696655,-1.2599321757,0.3942933697\H,-0.4523965775,-1.9123079148,0.2548831146\H,-0.7391783491,-0.5398142982,-1.4897662211\H,0.8505504891,1.223633384,-2.0421965645\H,2.1986654963,0.2852164005,-1.4375321118\H,-2.2969422747,0.9965297322,-0.1780715661\H,-1.9996079001,-0.6442313986,1.79451

29033\H,0.1188190796,-0.3075467807,3.1412287442\H,-0.4590433897,2.7250
513833,-0.3685286257\O,-0.1260880135,2.6217683105,1.6327328148\C,0.029
9582475,1.7851475203,2.6843611129\O,0.2002838481,2.2002292097,3.799902
6875\H,0.5928743237,-1.2760030896,-2.3401414713\H,2.1066951439,0.50073
38918,1.8772248621\H,1.810677714,1.9589041869,0.1686600527\N,0.8579474
233,-3.1122898062,-0.7554436272\C,2.1934602107,-3.2231777758,-1.318000
0592\H,2.2581704465,-4.1405505371,-1.9109806134\H,2.3998228652,-2.3793
743561,-1.9830843236\H,2.9895726195,-3.2608502296,-0.5534430491\C,0.61
27377152,-4.1815502468,0.1953628171\H,-0.4103730345,-4.1114030288,0.57
58634772\H,0.7207163467,-5.1453869901,-0.3116047191\H,1.3071397521,-4.
1775459699,1.0553035034\Version=ES64L-G09RevE.01\State=1-A\HF=-711.72
78931\RMSD=3.416e-09\RMSF=5.450e-06\Dipole=0.1543265,-1.2390614,-1.466
5668\Quadrupole=8.041408,-2.7038939,-5.3375141,-0.0282744,-0.2037265,-
12.9568416\PG=C01 [X(C13H19N1O2)]\@

5a(iv) [product]

1\1\GINC-R764\FOpt\RM062X\6-31+G(d,p)\C13H20N1O2(1+)\ROOT\07-Aug-2017\O
\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdi
sk=2147483648\|a6\|1,1\C,1.3262994775,0.2854571532,1.1984402513\C,0.91
70538065,1.2266983274,0.0305140066\C,1.6489003743,-1.1494954448,0.7420
513711\C,0.5725702053,-1.7499157665,-0.1620081318\C,0.2203792836,-0.83
75421549,-1.3610262758\C,0.936958393,0.5205321795,-1.326854715\C,0.218
8781483,0.3565075738,2.3012656639\C,-0.4373146263,1.8726665843,0.41270
7243\C,-1.4805410449,0.8211371735,0.7006868282\C,-1.1351615142,0.02539
56126,1.7157353651\H,1.7959936982,-1.7639016205,1.6349335423\H,2.60444
47633,-1.1291774367,0.1986863374\H,-0.321893693,-1.9748507206,0.426722
1156\H,-0.8628897419,-0.6963328823,-1.392565485\H,0.499800946,1.166897
9989,-2.0947793067\H,1.9840203185,0.3795119341,-1.6180913727\H,-2.4211
326434,0.7770104867,0.1620608551\H,-1.7668292406,-0.749474108,2.139607
4156\H,0.4841667301,-0.223667489,3.1851297809\H,-0.7519300767,2.616227
0799,-0.3192987445\O,-0.1823559964,2.6137393636,1.6272625272\C,0.17169
60922,1.8372151576,2.6795842084\O,0.444369577,2.2965621733,3.750451998
\H,0.4921925037,-1.3267499758,-2.3053440516\H,2.2438469213,0.662373318
2,1.6600716385\H,1.6249829749,2.0594711845,-0.0202449482\N,1.007330394
7,-3.1225336588,-0.6907279746\H,1.7290841643,-2.9499146312,-1.39938619
18\C,1.604179958,-4.0177893801,0.3502819316\H,1.7618632269,-5.00214426
06,-0.0901199639\H,2.5526111947,-3.6086575319,0.6905607462\H,0.9012660
735,-4.0906765578,1.1817538272\C,-0.1340409496,-3.8263368061,-1.359983
4243\H,-0.5948373662,-3.168245006,-2.0935571307\H,0.2406734249,-4.7267
009352,-1.8462734948\H,-0.8583827576,-4.0920729343,-0.5888634419\Vers
ion=ES64L-G09RevE.01\State=1-A\HF=-712.1024265\RMSD=9.223e-09\RMSF=6.9
42e-06\Dipole=0.6965595,-5.3618834,-3.385914\Quadrupole=-3.4555784,12.
8454909,-9.3899125,-4.9967424,-0.8951737,0.0035951\PG=C01 [X(C13H20N1O
2)]\@

3b(ii) [product]

1\1\GINC-R304\FOpt\RM062X\6-31+G(d,p)\C11H11O4(1-)\ROOT\07-Aug-2017\O
\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk
=1610612736\|a2\|1,1\C,1.4015393466,0.1559069941,1.3669041302\C,1.260
0697088,1.1141361164,0.1459383723\C,1.40927666,-1.2626106279,0.7726156
623\C,1.1643511121,0.2010007377,-1.0885397446\H,0.9724588056,-2.002299
821,1.451273203\H,2.4301666264,-1.5786223194,0.5261331121\H,0.52703781
9,0.6206554582,-1.8735301907\H,2.1563311228,0.0084555292,-1.5154422839
\C,2.6873583354,0.5566281983,2.1628892999\C,2.4599235619,2.0804454475,
0.1747769734\C,3.7461002319,1.2930490975,0.161168949\C,3.8682942789,0.
4927513726,1.219807042\H,2.8119202951,-0.0270982846,3.0746493283\H,2.4
052148159,2.8472044879,-0.5984664729\H,4.4495275084,1.3487076839,-0.66
14209662\H,4.6985675878,-0.1838071324,1.3897870551\O,2.3745665337,2.80
92061213,1.4358657594\C,2.4939278391,2.0191847589,2.5235157441\O,2.420
7907376,2.4785798057,3.6383770433\C,0.6502713438,-1.1457234513,-0.5574
956933\H,-0.4318140505,-1.1040136302,-0.380434708\H,0.5454025813,0.282
067179,2.0394323305\H,0.3568409473,1.7260592737,0.2517805554\C,0.95721
29217,-2.3317490175,-1.5276345108\O,-0.0255833303,-3.0175566872,-1.885
6729117\O,2.1696416597,-2.4546962902,-1.8304040784\Version=ES64L-G09R
evE.01\State=1-A\HF=-726.4997406\RMSD=4.954e-09\RMSF=4.296e-06\Dipole=
1.3305772,3.4284966,2.1280249\Quadrupole=19.093556,-15.1732572,-3.9202
988,-11.791565,-8.4492021,-36.5183876\PG=C01 [X(C11H11O4)]\@

3b(i) [product]

1\1\GINC-R346\FOpt\RM062X\6-31+G(d,p)\C11H12O4\ROOT\07-Aug-2017\0\#\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=161
0612736\|a5\|0,1\C,1.4355254462,0.1288582858,1.368543899\C,1.231822162
,1.0908260397,0.1578822485\C,1.4671682838,-1.2899747679,0.7779512867\C
,1.1230637213,0.1957748361,-1.0872924644\H,1.0549141666,-2.0443065188,
1.4519839271\H,2.4962154508,-1.5748487109,0.5273931287\H,0.443712874,0
.5976230121,-1.8432093528\H,2.1011752075,0.0528359068,-1.5597085187\C,
2.7302148988,0.5541108292,2.1278281727\C,2.4052670596,2.0917644205,0.1
599509409\C,3.7161081979,1.3452092961,0.108874797\C,3.8908346282,0.540
5248949,1.1578061239\H,2.8942333673,-0.0294090469,3.0331139396\H,2.306
0075347,2.8585379229,-0.6080821934\H,4.4176391439,1.4654434317,-0.7086
098199\H,4.7666138214,-0.0771496301,1.3247992783\O,2.3178863309,2.8014
245062,1.422303993\C,2.4933446239,2.0108794571,2.506723695\O,2.4290609
517,2.4513227371,3.6230496808\C,0.6606284607,-1.1540959085,-0.53300248
62\H,-0.4093748847,-1.1399941413,-0.2947678055\H,0.5938427619,0.219816
5646,2.0626362082\H,0.3154494731,1.6737783378,0.2943404758\C,0.9214275
122,-2.3120899793,-1.4612212976\O,1.6830950429,-2.3089394249,-2.397744
9135\O,0.2247543214,-3.4089049028,-1.1002667509\H,0.4669094421,-4.1219
68447,-1.7115321923\|Version=ES64L-G09RevE.01\|State=1-A\|HF=-727.046980
3\|RMSD=8.338e-09\|RMSF=1.027e-05\|Dipole=-0.2928023,-1.2778444,-1.015420
2\|Quadrupole=7.8069658,0.6754017,-8.4823676,-0.0334399,0.8225788,-11.4
917061\|PG=C01 [X(C11H12O4)]\|@

3b(iii) [product]

1\1\GINC-R347\FOpt\RM062X\6-31+G(d,p)\C12H17N1O2\ROOT\07-Aug-2017\0\#\#
M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=1
610612736\|a3\|0,1\C,1.3632483204,0.1927326424,1.3874912235\C,1.177163
6284,1.1335557805,0.1598579526\C,1.3602990917,-1.2351324135,0.82303591
25\C,1.0497602739,0.2150014862,-1.0639908597\H,0.9316389541,-1.9493623
116,1.5308010511\H,2.3782061363,-1.5619679382,0.5748481183\H,0.3739022
034,0.629095572,-1.8165905453\H,2.027315375,0.0454612393,-1.5340163449
\C,2.6699409731,0.6042289954,2.1348823776\C,2.3704163235,2.1113080817,
0.1404385091\C,3.6662000901,1.3387077757,0.1001322105\C,3.8268817761,0
.5489023978,1.1624928163\H,2.8246906009,0.032871411,3.0495327274\H,2.2
845845607,2.8663326815,-0.6409350617\H,4.367999048,1.4298964808,-0.720
9453848\H,4.6892108844,-0.0853158256,1.337234811\O,2.3010715807,2.8456
357187,1.3898909073\C,2.4652301531,2.0714060416,2.4880526067\O,2.41386
23625,2.5348408414,3.5961464631\C,0.5742703118,-1.1307926486,-0.493069
71\H,-0.5105019181,-1.056458898,-0.2576751373\H,0.5287144079,0.3205655
045,2.0842796006\H,0.2733542324,1.7385106814,0.2835919232\N,0.81250444
77,-2.2507614219,-1.3945455243\C,0.4249394273,-3.514892243,-0.78571849
4\H,0.5954275881,-4.3259328074,-1.4981811232\H,1.0309412236,-3.7145753
066,0.1001792146\H,-0.642406162,-3.52998315,-0.4924821324\C,0.11133755
77,-2.0746058494,-2.6578937576\H,-0.9822869049,-1.9715940755,-2.520484
7613\H,0.4801415632,-1.1895210949,-3.1800856925\H,0.2955758891,-2.9417
033477,-3.2971258967\|Version=ES64L-G09RevE.01\|State=1-A\|HF=-672.43820
74\|RMSD=3.860e-09\|RMSF=5.678e-06\|Dipole=-0.263283,-1.3913532,-1.537765
3\|Quadrupole=6.5563991,-2.9327951,-3.6236039,-0.6426446,-0.7006355,-11
.2478026\|PG=C01 [X(C12H17N1O2)]\|@

3b(iv) [product]

1\1\GINC-R239\FOpt\RM062X\6-31+G(d,p)\C12H18N1O2(1+)\ROOT\08-Aug-2017\
0\#\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdi
sk=1610612736\|a6\|1,1\C,1.5910863715,0.1059840331,1.5159961012\C,1.03
50878012,0.9891417611,0.3569254196\C,1.7109383943,-1.3189138782,0.9482
087952\C,0.82760091,0.0515175693,-0.8447450563\H,1.5233614441,-2.08158
55376,1.7069856175\H,2.7193998583,-1.4747223846,0.5380165586\H,-0.0382
501767,0.3343191965,-1.4471286898\H,1.7187642219,0.0636485897,-1.48960
33672\C,2.9360321706,0.7194175818,2.0092085627\C,2.0398994447,2.142355
8909,0.1297768347\C,3.4109120014,1.5791748655,-0.1620620314\C,3.887599
7472,0.8366697355,0.8398306728\H,3.3422569851,0.1933782042,2.872382939
4\H,1.6924392109,2.861074918,-0.6120583427\H,3.944217966,1.8045838766,
-1.0788810917\H,4.8721369296,0.381150884,0.8580452407\O,2.075765951,2.
8634890314,1.3781352951\C,2.5662153962,2.1441157828,2.4208589973\O,2.6
444037398,2.6000968892,3.5235970277\C,0.6972173924,-1.332924565,-0.200

2443061\H,-0.3209270525,-1.5076361747,0.1672722925\H,0.8905187225,0.1059448174,2.3558703255\H,0.084617764,1.4432092457,0.650320573\H,1.9095383949,-2.3078263357,-1.5442051567\N,0.9584152344,-2.4541904636,-1.1862653626\C,0.9232319539,-3.800853917,-0.532838605\H,1.0991679214,-4.5643799902,-1.2901885604\H,1.6937778992,-3.8499416452,0.2340211802\H,-0.063487607,-3.9357648662,-0.0872182759\C,0.0229989748,-2.4097662876,-2.3543504229\H,-0.9964391217,-2.4982367001,-1.9758004215\H,0.1493861208,-1.4665648507,-2.8822387427\H,0.248955036,-3.2436752763,-3.0184430009\Version=ES64L-G09RevE.01\State=1-A\HF=-672.8094256\RMSE=6.093e-09\RMSEF=1.302e-05\Dipole=-1.4342486,-5.0403056,-3.8043911\Quadrupole=-2.146156,7.211872,-5.065716,6.2647454,4.0535891,3.0837518\PG=C01 [X(C12H18N1O2)]\@

5c(ii) [product]

1\1\GINC-R767\FOpt\RM062X\6-31+G(d,p)\C12H13O4(1-)\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=2147483648\@5\0,1\C,1.4590900414,0.1307110646,1.2297952222\C,1.3286535314,1.1323205907,0.0429047823\C,1.6368649573,-1.3124618709,0.7544557076\C,0.5281761887,-1.753017746,-0.2156483978\C,0.2437650448,-0.6861010022,-1.2939514149\C,1.3003221622,0.4219460303,-1.3116114848\H,1.6535919278,-2.0024714694,1.6031984903\H,2.6081323444,-1.4113376696,0.2516968148\H,-0.3781087506,-1.931880801,0.3778160556\H,-0.7376070409,-0.2191901283,-1.1244372396\H,1.0868728628,1.1520438108,-2.1039638374\H,2.2806316213,-0.0173903111,-1.5348777806\C,2.6589449385,0.6000914963,2.1248558441\C,2.4657280873,2.1659535996,0.1762504768\C,3.7959654952,1.45780617,0.2175404793\C,3.8995584245,0.6332167612,1.2605906706\H,2.7559005078,-0.0098851561,3.0224398856\H,2.4048844573,2.9475986144,-0.5822356757\H,4.5487705946,1.592949015,-0.5507957461\H,4.7584615638,0.0058598058,1.4730540888\O,2.2619347685,2.8504388153,1.4437574289\C,2.3530628189,2.0328611497,2.5154391384\O,2.1742448532,2.45134138,3.6336854608\H,0.2205085683,-1.196316234,-2.2607617803\H,0.5536021426,0.1851260895,1.847076823\H,0.3923586291,1.6957151343,0.1516478431\C,0.9586394099,-3.1493519689,-0.7974045737\O,1.195725596,-3.2023208242,-2.0261256889\O,1.0502472538,-4.0508763459,0.0676964076\Version=ES64L-G09RevE.01\State=1-A\HF=-765.7967595\RMSE=6.180e-09\RMSEF=1.962e-06\Dipole=1.1620093,4.4656236,0.7094786\Quadrupole=27.6101563,-31.2001846,3.5900283,-8.6093762,-3.7814238,-28.1652296\PG=C01 [X(C12H13O4)]\@

5c(i) [product]

1\1\GINC-R943\FOpt\RM062X\6-31+G(d,p)\C12H14O4\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=2147483648\@2\0,1\C,1.4717926896,0.1253112794,1.2391667136\C,1.3133119678,1.1184461328,0.0481737771\C,1.6481294139,-1.3202447295,0.7732708061\C,0.4937727839,-1.7462680375,-0.1622851948\C,0.2144339079,-0.7051786665,-1.2704160555\C,1.2687682384,0.4035537301,-1.3023243931\H,1.6877753268,-1.9928396008,1.6355071407\H,2.6015414361,-1.4190955182,0.2401741649\H,-0.3977916922,-1.8936079657,0.4584077655\H,-0.7666570674,-0.2497910403,-1.0954343779\H,1.0282827084,1.1213611012,-2.0942719702\H,2.2505755345,-0.0209526869,-1.5453309937\C,2.6872067895,0.5937198629,2.1047122128\C,2.4479704459,2.1587382152,0.1586768303\C,3.7842152753,1.4586014418,0.1779369229\C,3.9141169312,0.6373877474,1.2208755693\H,2.8033360575,-0.0085969627,3.0053672521\H,2.3683567123,2.9358935999,-0.6017204419\H,4.5342129411,1.6215185336,-0.5875832717\H,4.7951573922,0.043032013,1.4376249485\O,2.2539845685,2.8396349473,1.4233097448\C,2.3712675048,2.0285797654,2.4992883065\O,2.2042676227,2.4369191289,3.6174646058\H,0.1712396096,-1.210653537,-2.2379272079\H,0.5787617358,0.174575963,1.8737563922\H,0.376121328,1.6748145663,0.1722547236\C,0.8446821578,-3.1018378219,-0.7381343702\O,1.1479870851,-3.3366694922,-1.8825449055\O,0.8235316455,-4.0622864932,0.2096689545\H,1.0868819496,-4.8939174757,-0.2137386488\Version=ES64L-G09RevE.01\State=1-A\HF=-766.344534\RMSE=3.966e-09\RMSEF=2.981e-06\Dipole=0.0716176,-1.1243855,-1.0033471\Quadrupole=9.2700944,-0.5116543,-8.7584401,-0.8757969,-0.7013224,-15.1763244\PG=C01 [X(C12H14O4)]\@

5c(iii) [product]

1\1\GINC-R2813\FOpt\RM062X\6-31+G(d,p)\C13H19N1O2\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=

2147483648\|a5\|0,1\C,1.6555606946,0.0513461772,1.1925271558\C,1.24714
31108,1.1444581071,0.1582103341\C,1.7494344852,-1.338872187,0.56032339
43\C,0.4299294576,-1.7221548572,-0.1379104556\C,-0.0534247318,-0.59166
87965,-1.0863493786\C,0.9530010657,0.5533713957,-1.2211945091\H,1.9924
945735,-2.0760585723,1.3346571163\H,2.5730935729,-1.3501700458,-0.1630
611282\H,-0.3250531189,-1.8492597523,0.6487315505\H,-0.995428691,-0.18
09886063,-0.7048542949\H,0.5530197926,1.3315557191,-1.8813142057\H,1.8
819198208,0.1920962143,-1.6812022782\C,3.0107279454,0.4830761162,1.843
5049793\C,2.3612795636,2.2122963359,0.146615292\C,3.687247894,1.564033
0176,-0.1659497663\C,4.0357610295,0.6533898562,0.7442944029\H,3.314919
6466,-0.1961380917,2.639482219\H,2.1181051226,3.0536903196,-0.50270621
21\H,4.267542253,1.8261350721,-1.0433121198\H,4.9522232794,0.073525112
2,0.7232920263\C,2.4109638659,2.7650919759,1.4856535444\C,2.7562112749
,1.8621235195,2.431856642\O,2.8092482584,2.1594263199,3.5957416778\H,-
0.2873968082,-1.0257076438,-2.0624474107\H,0.9069418808,0.0167521351,1
.9934769344\H,0.3414128147,1.6512239773,0.513309766\N,0.4641167807,-3.
0079815701,-0.8442525564\C,1.4892714249,-3.1017707476,-1.8702001615\H,
1.2902582776,-3.9765132406,-2.4966100217\H,1.4685118039,-2.2176425811,
-2.5138549233\H,2.5100053897,-3.2066958564,-1.4612607829\C,0.525595577
5,-4.1518135547,0.0478541434\H,-0.2694860217,-4.0810354803,0.795665736
8\H,0.3681452094,-5.0674463139,-0.5303304116\H,1.4926215053,-4.2504644
731,0.5737507014\|Version=ES64L-G09RevE.01\|State=1-A\|HF=-711.7327744\|R
MSD=6.499e-09\|RMSF=3.351e-06\|Dipole=0.0408416,-1.1373366,-1.6145284\|Qu
adpole=5.6315399,-0.9303764,-4.7011635,-3.8343609,-4.7250627,-12.024
3147\|PG=C01 [X(C13H19N1O2)]\|@

5c(iv) [product]

1\1\GINC-R232\|FOpt\|RM062X\|6-31+G(d,p)\|C13H20N1O2(1+)\|ROOT\07-Aug-2017\|
0\|#M062X\|6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdi
sk=2147483648\|a5\|1,1\C,1.6536183128,0.0545028398,1.2111533509\C,1.24
45144971,1.1435839534,0.171461355\C,1.7308710047,-1.3464894469,0.58792
03952\C,0.3927678332,-1.6813992233,-0.0656396528\C,-0.0949304255,-0.58
34650074,-1.0426682947\C,0.9237430209,0.5490846977,-1.2007278715\H,1.9
815338095,-2.072855492,1.3680920525\H,2.5368578993,-1.3527904037,-0.15
3616947\H,-0.35639551,-1.8390312128,0.7171812992\H,-1.029409343,-0.167
079221,-0.6539013714\H,0.5080638946,1.3194260224,-1.8569028233\H,1.839
8842277,0.1831419733,-1.6816181003\C,3.0269215056,0.461564356,1.832511
1564\C,2.3770099261,2.1945102241,0.1356327206\C,3.6894111887,1.5235612
904,-0.1918113586\C,4.0397479975,0.6133262606,0.7190679146\H,3.3318738
548,-0.2125736402,2.6327790033\H,2.1360731731,3.03328306,-0.5172763641
\H,4.2751298678,1.7938718252,-1.0631252524\H,4.9637780473,0.0451102062
,0.7059909366\O,2.4435301864,2.7496069115,1.466561484\C,2.7910399945,1
.8509060587,2.4187952805\O,2.8554119052,2.1429502254,3.5780566602\H,-0
.344709647,-1.0115804134,-2.0217792566\H,0.9187168254,0.0296187087,2.0
24358223\H,0.3527270871,1.6659780316,0.5366374171\N,0.4368977981,-3.03
25276628,-0.787162549\H,-0.4660199467,-3.1063013494,-1.2668877296\C,1.
4963138195,-3.1253466495,-1.8412035657\H,1.2940311167,-4.0000764134,-2
.4593767236\H,1.4812792224,-2.2231429278,-2.4520848642\H,2.4639977019,
-3.2352877887,-1.3541589208\C,0.5225147513,-4.193967121,0.1524742918\H
,0.2855346316,-4.1227403932,0.8803340705\H,0.4322716502,-5.1162822057
,0.4217633167\H,1.4879193843,-4.1670450726,0.655856351\|Version=ES64L
-G09RevE.01\|State=1-A\|HF=-712.1066203\|RMSD=7.729e-09\|RMSF=1.614e-06\|Di
pole=-2.0449801,-5.2877058,-3.4071447\|Quadrupole=-1.2033717,13.7941699
,-12.5907982,9.0736774,1.4900147,-0.5353045\|PG=C01 [X(C13H20N1O2)]\|@

5b(ii) [product]

1\1\GINC-R822\|FOpt\|RM062X\|6-31+G(d,p)\|C12H13O4(1-)\|ROOT\07-Aug-2017\|
0\|#M062X\|6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk
=2147483648\|a6\|1,1\C,1.1722298843,0.135061402,1.3036516883\C,0.9638
199731,1.1776021162,0.1669798804\C,1.4543672418,-1.279127422,0.7806439
326\C,0.5047507732,-1.7831834501,-0.3173745641\C,0.2897963948,-0.74223
77813,-1.4321029011\C,1.0867945297,0.5515128211,-1.2290581273\C,-0.052
1789459,0.2308014198,2.2434945107\C,-0.4049484483,1.9058586785,0.41530
04049\C,-1.5222127226,0.893549857,0.5196297898\C,-1.3329861023,-0.0026
517074,1.4884137703\H,1.4516352288,-2.0040973717,1.6013547845\H,2.4774
21379,-1.2837039299,0.3803856675\H,-0.4553295324,-2.024940786,0.153594
1104\H,-0.7768315816,-0.5018935132,-1.5246162213\H,0.8109644849,1.2992

387028,-1.9852171578\H,2.1490269725,0.3299495767,-1.3930968829\H,-2.37
07405905,0.9095190609,-0.1556624031\H,-1.9866021882,-0.8383409535,1.70
89429265\H,0.0625862885,-0.3996091461,3.125146854\H,-0.5806014383,2.69
376749,-0.3174608245\C,-0.2588338171,2.5262578736,1.7937030649\O,-0.06
5879604,1.5998564692,2.7529134702\O,-0.2724750861,3.7062113712,2.05375
82786\H,0.6035478496,-1.2098972034,-2.3708487202\H,2.0225184438,0.4497
205999,1.9217585013\H,1.7303247229,1.9576316954,0.2533647012\C,1.07558
90662,-3.1619611437,-0.8184140368\O,1.0829752176,-4.0510605329,0.06529
32082\O,1.4795246063,-3.2176791933,-2.0017587053\Version=ES64L-G09Rev
E.01\State=1-A\HF=-765.793032\RMSD=3.549e-09\RMSF=5.759e-06\Dipole=-1.
3881539,3.798444,1.238071\Quadrupole=25.594595,-35.5384788,9.9438838,1
4.7190292,7.7291951,-26.3180822\PG=C01 [X(C12H13O4)]\@

5b(i) [product]

1\1\GINC-R823\FOpt\RM062X\6-31+G(d,p)\C12H14O4\ROOT\07-Aug-2017\0\#M0
62X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=214
7483648\A4\0,1\C,1.2289724411,0.1792373833,1.2675176994\C,0.93588527
72,1.205581003,0.1354486145\C,1.5642666237,-1.2227805309,0.7444936521\
C,0.5906412271,-1.7514376393,-0.3344070044\C,0.3187875097,-0.729241660
9,-1.4577767562\C,1.0683554553,0.5920165442,-1.2631925247\C,0.03752645
24,0.2251001634,2.2555224301\C,-0.4629497925,1.8539264768,0.4171276204\
C,-1.5224868374,0.7879527979,0.5733961496\C,-1.2586229074,-0.08109430
01,1.5505108109\H,1.6068257063,-1.9337395288,1.5765569859\H,2.57289765
99,-1.1877969622,0.3147778411\H,-0.3462652235,-2.0223866616,0.16297958
3\H,-0.7571247498,-0.5403385495,-1.5133647232\H,0.7369236947,1.3182675
879,-2.0137782962\H,2.1352312077,0.4242171893,-1.454353367\H,-2.410803
7767,0.7719545716,-0.0492788008\H,-1.8882730187,-0.9168931042,1.834879
9513\H,0.2163741522,-0.3905906447,3.1372683555\H,-0.7046023585,2.62334
99724,-0.31572331\C,-0.3003613779,2.5000815769,1.7863098563\O,-0.01473
96114,1.5891663561,2.7462828841\O,-0.3658668714,3.6745450179,2.0326155
24\H,0.6158977566,-1.164973703,-2.4153013309\H,2.092296699,0.523570991
9,1.8471043903\H,1.6614567718,2.0233215717,0.2025190581\C,1.1637444861
,-3.0463943025,-0.8722874276\O,1.6328607901,-3.2259969856,-1.969545472
6\O,1.1271766739,-4.0246315261,0.0583263022\H,1.5335989404,-4.81272910
48,-0.3339956952\Version=ES64L-G09RevE.01\State=1-A\HF=-766.3401371\R
MSD=6.426e-09\RMSF=8.449e-06\Dipole=0.0059285,-1.5958763,-0.4551384\Qu
adrupole=8.2892375,-5.2329312,-3.0563063,2.9308144,4.4985782,-13.44272
91\PG=C01 [X(C12H14O4)]\@

5b(iii) [product]

1\1\GINC-R2477\FOpt\RM062X\6-31+G(d,p)\C13H19N1O2\ROOT\07-Aug-2017\0\
#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=
2147483648\A3\0,1\C,1.1428161433,0.1690564015,1.3605804286\C,0.96017
92746,1.1890356744,0.199144152\C,1.4745700516,-1.2477363285,0.87213483
83\C,0.5650179471,-1.7855069652,-0.2518947253\C,0.3794392755,-0.752481
2819,-1.390388882\C,1.1580081843,0.5486685172,-1.181025319\C,-0.112552
3475,0.2648733176,2.2621476675\C,-0.4301688978,1.8902045414,0.38133986
76\C,-1.5352759154,0.8638021996,0.4747587927\C,-1.367933632,-0.0040551
099,1.4737445439\H,1.4612652568,-1.9387115012,1.7246792766\H,2.5098845
391,-1.2302514622,0.5115461691\H,-0.4208792527,-1.9812147572,0.1836290
291\H,-0.686471288,-0.5305143325,-1.4977816719\H,0.8973523414,1.273584
556,-1.96092161\H,2.2307720969,0.3475068676,-1.2999672008\H,-2.3786797
689,0.8708075901,-0.2075528295\H,-2.0427236946,-0.8165396442,1.7188933
694\H,-0.0153424332,-0.3467609905,3.1594840738\H,-0.594960511,2.659987
2523,-0.3722468764\C,-0.3363142189,2.5448413534,1.7528013818\O,-0.1526
121052,1.6357042763,2.7379738394\O,-0.3741972199,3.724240529,1.9833953
347\H,0.6822086509,-1.2128407049,-2.3356329011\H,1.9703157064,0.501279
7864,1.9971020899\H,1.708385552,1.982473964,0.3023978375\N,0.995436789
4,-3.0798214372,-0.7978222221\C,0.7765150304,-4.190667685,0.1104906398
H,0.9488706568,-5.1308068265,-0.4225253934\H,1.4436478362,-4.18019494
32,0.99178928\H,-0.2599719008,-4.1843563944,0.4602664774\C,2.352418796
8,-3.1022139694,-1.3176175549\H,2.4850075121,-3.9955152591,-1.93557384
16\H,2.5347829262,-2.2280932246,-1.9495513398\H,3.1248126181,-3.123329
0095,-0.5284277214\Version=ES64L-G09RevE.01\State=1-A\HF=-711.727956\
RMSD=6.473e-09\RMSF=5.148e-06\Dipole=0.3644757,-1.753885,-0.8503056\Qu
adrupole=8.1354041,-9.2060284,1.0706242,2.1296481,0.8044435,-11.403626
4\PG=C01 [X(C13H19N1O2)]\@

5b(iv) [product]

1\1\GINC-R904\FOpt\RM062X\6-31+G(d,p)\C13H20N1O2(1+)\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=2147483648\|a2\|1,1\C,1.0638639935,0.1250368953,1.4098281931\C,0.9877094908,1.1678105639,0.2594107142\C,1.3564779014,-1.3076103212,0.9282716163\C,0.4753602232,-1.7501543267,-0.2420259284\C,0.4650997785,-0.7306661052,-1.4061162986\C,1.2695595062,0.5409916059,-1.1077988203\C,-0.2346940541,0.2599111031,2.2472511827\C,-0.3881806447,1.9059656217,0.3588660157\C,-1.530721532,0.917563998,0.3806534718\C,-1.4532011351,0.0398624563,1.3843688712\H,1.2386315398,-1.9859437466,1.779165417\H,2.410816821,-1.3542617953,0.6219818998\H,-0.5426788299,-1.9387110366,0.111401603\H,-0.5705946829,-0.4771834311,-1.6468785684\H,1.0826443559,1.2712899827,-1.9008689891\H,2.339950126,0.3083803876,-1.1594647375\H,-2.3514962875,0.9798511896,-0.3270270154\H,-2.1969500892,-0.7164897518,1.6132382375\H,-0.2097035402,-0.3634344249,3.1418701186\H,-0.4822262803,2.6870308208,-0.3949596799\C,-0.3529483305,2.5498199038,1.7435573684\O,-0.242511944,1.6185816789,2.7282848775\O,-0.3682248477,3.7217541203,1.9807913341\H,0.8870880632,-1.1814672233,-2.313504952\H,1.8779580656,0.3943558555,2.0893330877\H,1.7533683786,1.9322292898,0.4226655868\N,0.9273119263,-3.1147601577,-0.7770548771\H,1.7989633611,-2.9542997268,-1.2941808499\C,-0.07897224,-3.6758489538,-1.7356166678\H,0.3367594627,-4.5673973519,-2.2045431589\H,-0.9718436104,-3.9354845899,-1.1652992254\H,-0.3229497078,-2.9333783543,-2.49239479\C,1.2158412949,-4.125190735,0.2892009017\H,1.407048115,-5.0861199677,-0.1881347383\H,2.0863023692,-3.8185091383,0.8644289034\H,0.3395739834,-4.1991313352,0.9353378964\|Version=ES64L-G09RevE.01\State=1-A\HF=-712.1019624\RMSD=7.826e-09\RMSF=1.467e-05\Dipole=1.1004211,-5.8398321,-2.8338145\Quadrupole=-3.9527884,8.4696602,-4.5168718,-3.3042874,0.0279256,1.5206546\PG=C01 [X(C13H20N1O2)]\|@

5d(ii) [product]

1\1\GINC-R764\FOpt\RM062X\6-31+G(d,p)\C12H13O4(1-)\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=2147483648\|a5\|1,1\C,1.4159709364,0.1185605801,1.2368347596\C,1.2974211495,1.1562743797,0.0799839158\C,1.5958486166,-1.3124505683,0.7280777009\C,0.50573921,-1.7069200035,-0.2795283017\C,0.3314655604,-0.6428529616,-1.3850655143\C,1.3626208163,0.4864627698,-1.2940620035\H,1.576546515,-2.0287772593,1.5549483081\H,2.5786222197,-1.4123386551,0.2474086853\H,-0.4311931729,-1.8156759843,0.2832886414\H,-0.671798724,-0.1965248101,-1.3313436667\H,1.1847351987,1.2385462378,-2.074188369\H,2.367246043,0.0800906325,-1.4648468323\C,2.5802206822,0.5753895627,2.1406960975\C,2.4058757169,2.2447443863,0.2778731027\C,3.750184837,1.5541516904,0.3343501057\C,3.843312322,0.6620528964,1.3212391249\H,2.6744971946,-0.0417935778,3.0341359192\H,2.3393653358,3.0350774952,-0.4700433606\H,4.5311001875,1.7634231199,-0.3889200989\H,4.698047676,0.0219728445,1.5079883861\C,2.1524390724,2.8313485064,1.6536469279\O,2.2513141277,1.9074945969,2.630252903\O,1.8626158405,3.9774310363,1.901617657\H,0.4216290018,-1.157385398,-2.3463596404\H,0.5081589621,0.160938209,1.8521690329\H,0.3296472442,1.6685415906,0.1573735548\C,0.8586150824,-3.1437809954,-0.8154280648\O,1.0894394267,-3.2542326809,-2.040848953\O,0.8951909217,-4.0196086405,0.0803399825\|Version=ES64L-G09RevE.01\State=1-A\HF=-765.7970875\RMSD=4.299e-09\RMSF=2.302e-06\Dipole=1.3986024,4.141637,1.2009161\Quadrupole=28.5314928,-39.9754132,11.4439204,-9.0194571,-3.1476684,-26.4954687\PG=C01 [X(C12H13O4)]\|@

5d(i) [product]

1\1\GINC-R270\FOpt\RM062X\6-31+G(d,p)\C12H14O4\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=2147483648\|a5\|0,1\C,1.3882124296,0.1119142094,1.2167524755\C,1.2948407737,1.1613133691,0.067876886\C,1.5361351686,-1.3187204693,0.6996490473\C,0.4088235404,-1.6478758775,-0.3030216557\C,0.2988329455,-0.595486293,-1.4313181128\C,1.3556686826,0.5056550899,-1.3121343803\H,1.5040532949,-2.0282075542,1.5326228236\H,2.5078985949,-1.4390284898,0.2052301177\H,-0.526714649,-1.6996855076,0.2666133568\H,-0.695151391,-0.1362718899,-1.3971404897\H,1.1893823594,1.2619753989,-2.0868447005\H,2.35435141

7,0.0876832581,-1.4862478855\C,2.565429967,0.5287400714,2.1269953669\C
,2.4257536935,2.2191682491,0.2783737171\C,3.7568005773,1.5036022605,0.
3313693241\C,3.8318109608,0.6000995624,1.3097434267\H,2.6465197655,-0.
1036133607,3.0114160537\H,2.3752363481,3.0198973191,-0.4589803577\H,4.
5528371952,1.725325057,-0.371171701\H,4.6880851879,-0.0328535932,1.513
0187949\C,2.1739689991,2.7950556618,1.6628037294\O,2.2487685437,1.8493
120451,2.6287661026\O,1.8988123523,3.9361312898,1.9210944615\H,0.39114
28613,-1.0951906737,-2.3986901597\H,0.4828416979,0.1670941764,1.833354
1657\H,0.3376820723,1.6909390227,0.1474495149\C,0.6523012636,-3.040186
0825,-0.846965901\O,0.9990066502,-3.3220543449,-1.9679349536\O,0.46971
79736,-3.980634576,0.1041301298\H,0.6679587243,-4.8408023283,-0.297130
1968\Version=ES64L-G09RevE.01\State=1-A\HF=-766.3443716\RMSD=4.150e-0
9\RMSE=4.784e-06\Dipole=0.1574658,-1.5660313,-0.4680188\Quadrupole=9.5
693705,-6.3057281,-3.2636424,0.2431585,0.0686167,-14.1720318\PG=C01 [X
(C12H14O4)]\@

5d(iii) [product]

1\1\GINC-R2653\FOpt\RM062X\6-31+G(d,p)\C13H19N1O2\ROOT\07-Aug-2017\O\\
#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=
2147483648\|a5\|,1\C,1.6784184437,0.0872837786,1.1855519786\C,1.24251
13078,1.2354648924,0.2242960971\C,1.778366796,-1.2641628491,0.47676187
38\C,0.4539008656,-1.5897182791,-0.239515007\C,0.0476565795,-0.4472746
176,-1.2102947377\C,1.0236399545,0.7320209444,-1.2036746958\H,2.013528
6048,-2.0480438355,1.2072224362\H,2.6027483959,-1.2400666647,-0.245857
6529\H,-0.3161284862,-1.6615675717,0.5397229307\H,-0.9497405755,-0.084
8039012,-0.9370742042\H,0.634745934,1.5459069451,-1.8258527056\H,1.984
4454533,0.4309842198,-1.6399167765\C,3.0099695257,0.5163754408,1.83954
81026\C,2.3150017246,2.3700906009,0.2991807437\C,3.6649981877,1.783343
1049,-0.0471285343\C,4.0337673515,0.7924228079,0.7659842395\H,3.345023
785,-0.1941281941,2.5955474873\H,2.0341866122,3.2355369416,-0.30052860
72\H,4.2515059826,2.1526781154,-0.8814668562\H,4.9540455354,0.22526294
73,0.684278765\C,2.3670703395,2.7714157788,1.7648587812\O,2.7397450899
,1.7432136316,2.5616332411\O,2.0854650398,3.8485518601,2.2187236935\H,
-0.0491729684,-0.8568339274,-2.2197792023\H,0.9478341664,0.0027354429,
1.9995116597\H,0.2960819354,1.6598334434,0.5809600238\N,0.4252599487,-
2.8845705951,-0.9273497925\C,1.5059124754,-3.0739328479,-1.88065626\H,
1.2788762576,-3.9350089434,-2.5162356659\H,1.6045640374,-2.1964952422,
-2.5264718493\H,2.4830522231,-3.257749512,-1.3991833642\C,0.3379521767
,-4.0157110727,-0.0213980891\H,-0.5045855548,-3.8787587959,0.662244450
4\H,0.1608863545,-4.9270291975,-0.6005732365\H,1.2533335006,-4.1735578
486,0.5778887331\Version=ES64L-G09RevE.01\State=1-A\HF=-711.7328233\RM
SD=9.635e-09\RMSE=5.206e-06\Dipole=0.3009021,-1.6295824,-1.1805163\Qu
adrupole=6.5746624,-6.3245357,-0.2501267,-2.3798138,-3.0276152,-12.055
5229\PG=C01 [X(C13H19N1O2)]\@

5d(iv) [product]

1\1\GINC-R3180\FOpt\RM062X\6-31+G(d,p)\C13H20N1O2(1+)\ROOT\07-Aug-2017
\O\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxd
isk=2147483648\|a1\|,1\C,1.478915721,0.1808733612,1.2543012216\C,1.29
40791363,1.2268960788,0.1110817353\C,1.5933810763,-1.2547732309,0.7255
630875\C,0.3738691869,-1.5384209324,-0.1457274339\C,0.2353989666,-0.54
69470577,-1.3275000485\C,1.2811644777,0.5721007627,-1.2719681221\H,1.6
496464193,-1.9498430485,1.5708790953\H,2.5174128246,-1.3507898352,0.14
53334073\H,-0.5217625866,-1.4932343082,0.4825426524\H,-0.7674303643,-0
.1095421692,-1.3007951067\H,1.04880955,1.3186001568,-2.0368503456\H,2.
2762455274,0.1760499377,-1.5077674443\C,2.7242256164,0.6013632453,2.07
2027748\C,2.4244174296,2.2954934616,0.2427306254\C,3.7655327733,1.5984
450222,0.1950769062\C,3.924087714,0.6904925693,1.1601250449\H,2.879409
0167,-0.0365129625,2.9428621065\H,2.3080808925,3.1002019901,-0.4825174
512\H,4.5147309873,1.852576885,-0.5470082403\H,4.8144947892,0.09173750
65,1.3155680183\C,2.2622739325,2.8624583823,1.6486060017\O,2.419945668
8,1.9055321392,2.6012629711\O,1.9844131692,3.9916736867,1.9296768086\H
,0.3118676131,-1.0711807247,-2.2886048266\H,0.6260188774,0.2341803609,
1.9411706801\H,0.3370885758,1.7429714246,0.2514628341\N,0.364767338,-2
.9753738643,-0.6763232053\H,-0.3803748736,-2.9966915882,-1.3801723557\
C,1.6316731312,-3.3670829076,-1.3707707655\H,1.45540017,-4.2918918672,
-1.91999002\H,1.9301006762,-2.5742545325,-2.0564621167\H,2.4039233579,

-3.5248562883,-0.6190215705\C,-0.0003563243,-3.9813262502,0.3695466986
\\H,-0.9640085971,-3.7111283783,0.8006040844\\H,-0.058171321,-4.96580965
09,-0.0951451293\\H,0.7704994516,-3.9822173741,1.1391024548\\Version=ES
64L-G09RevE.01\\State=1-A\\HF=-712.1062206\\RMSD=9.562e-09\\RMSF=6.129e-06
\\Dipole=-1.6126878,-6.0424973,-2.6821627\\Quadrupole=-0.6336257,8.73407
18,-8.1004461,11.7874574,3.2272604,-0.3509328\\PG=C01 [X(C13H20N1O2)]\\
@

3c(ii) [product]

1\\1\\GINC-R267\\FOpt\\RM062X\\6-31+G(d,p)\\C11H11O4(1-)\\ROOT\\07-Aug-2017\\0\\
\\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk
=1610612736\\a4\\-1,1\\C,1.4903346147,0.8712574408,0.6088773886\\C,0.708
1850557,0.0973125741,1.7127064403\\C,1.4967800667,-0.0505557955,-0.6268
820488\\C,1.2080406211,-1.4782355107,-0.1332182084\\C,0.2743788417,-1.22
96715529,1.0607928227\\H,2.4334781776,0.0186844729,-1.1916472966\\H,0.67
17996026,0.231000753,-1.2909003634\\H,2.1295172625,-1.9830206964,0.1732
466007\\H,0.2683085623,-2.061275496,1.7754961389\\H,-0.7359347821,-1.121
5453659,0.6505243861\\C,2.893984124,1.1808959928,1.1711260061\\C,1.65262
66884,-0.0731286959,2.9491731852\\C,2.0855769748,1.3087708941,3.3900793
098\\C,2.7393661156,1.983150421,2.4419048236\\H,3.543025897,1.6461532673
,0.4282235229\\H,1.1929068137,-0.6712022854,3.7357274335\\H,1.856443762,
1.6910052619,4.3798717568\\H,3.1058384157,2.9999745633,2.5348399654\\C,2
.9119215185,-0.7723969903,2.4665035252\\O,3.5422626877,-0.0745049991,1.
4963881904\\O,3.3505761213,-1.8160513162,2.8778899728\\H,1.0184204506,1.
8346474783,0.3868718933\\H,-0.1548113315,0.6720794246,2.0646763194\\C,0.
5195971694,-2.3310643147,-1.2544594746\\O,-0.5979661525,-1.8939725078,-
1.6282442748\\O,1.1567057226,-3.3264070173,-1.6595750152\\Version=ES64L
-G09RevE.01\\State=1-A\\HF=-726.4934216\\RMSD=4.870e-09\\RMSF=6.259e-06\\Di
pole=1.1624113,4.8121732,3.8626549\\Quadrupole=3.9944893,1.5091473,-5.5
036366,-3.1278211,-18.026681,-16.9283534\\PG=C01 [X(C11H11O4)]\\@

3c(i) [product]

1\\1\\GINC-R934\\FOpt\\RM062X\\6-31+G(d,p)\\C11H12O4\\ROOT\\07-Aug-2017\\0\\#M0
62X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=161
0612736\\a4\\0,1\\C,1.4952615175,0.8851233676,0.5954463445\\C,0.68673660
34,0.1395424012,1.7029405098\\C,1.4918409755,-0.0392001464,-0.638776413
2\\C,1.1857819919,-1.4526987295,-0.0922440315\\C,0.2302204838,-1.1924493
481,1.076107536\\H,2.4311134303,-0.0067126773,-1.1974654304\\H,0.6861885
601,0.2657814554,-1.3164812004\\H,2.1159409914,-1.9256876332,0.23858363
91\\H,0.2217557963,-2.0151369405,1.7979111245\\H,-0.784349673,-1.0941098
564,0.6779993428\\C,2.9103209226,1.1446219163,1.1566504593\\C,1.61814047
63,-0.0461778467,2.9473897534\\C,2.1077918627,1.3192237525,3.3740553162
\\C,2.7887491538,1.9573784061,2.4216715653\\H,3.5786263746,1.5789567856,
0.4130068367\\H,1.1301885042,-0.6170542916,3.7366140202\\H,1.9042110914,
1.7117530079,4.3643411369\\H,3.2092208256,2.9525351367,2.5092556678\\C,2
.8238047306,-0.817953727,2.4426225617\\O,3.4897562299,-0.1462887355,1.4
738234983\\O,3.1591550892,-1.9220305783,2.7819379429\\H,1.050841355,1.85
48467122,0.3565812905\\H,-0.1709001054,0.7292099552,2.0352133092\\C,0.58
67849205,-2.3258826625,-1.1651318298\\O,-0.5780164697,-2.6271416421,-1.
2700152388\\O,1.5148257177,-2.7177458114,-2.0611489563\\H,1.0622766439,-
3.2491962702,-2.7343047549\\Version=ES64L-G09RevE.01\\State=1-A\\HF=-727
.0486835\\RMSD=8.567e-09\\RMSF=5.258e-06\\Dipole=-0.4335943,1.7802791,-0.
2556562\\Quadrupole=-8.1796376,2.9335547,5.2460829,1.7662008,-5.6685261
,5.181767\\PG=C01 [X(C11H12O4)]\\@

3c(iii) [product]

1\\1\\GINC-R1129\\FOpt\\RM062X\\6-31+G(d,p)\\C12H17N1O2\\ROOT\\07-Aug-2017\\0\\
\\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=
1610612736\\a1\\0,1\\C,1.5082891708,0.916680503,0.6253251675\\C,0.717677
1928,0.1646181271,1.7391419692\\C,1.534571571,-0.0273222706,-0.59128631
13\\C,1.2558271919,-1.4405886702,-0.0542667608\\C,0.3013899879,-1.183774
4432,1.1243179805\\H,2.4804559487,0.0427677034,-1.1373810529\\H,0.722508
4564,0.2317888803,-1.2813461987\\H,2.1981031558,-1.8865821672,0.3179879
448\\H,0.311571942,-1.9886103009,1.8664784054\\H,-0.7141868997,-1.109515
222,0.7170310461\\C,2.9107170536,1.2290875114,1.1913636226\\C,1.64735610
23,0.0212516558,2.9900174769\\C,2.0889178146,1.4080439204,3.4014910469\\
C,2.7541672268,2.0553481158,2.444092873\\H,3.5691140678,1.6748899786,0.

4455322277\H,1.1739101452,-0.5547312047,3.7844856825\H,1.8656342477,1.8074168937,4.3848250557\H,3.139454052,3.0656690777,2.5201614611\C,2.8849398873,-0.7145534584,2.5074563053\O,3.5328211613,-0.0356245111,1.532511878\O,3.2636203438,-1.7945644628,2.8780145746\H,1.0373322494,1.8702413357,0.3719302947\H,-0.1571410405,0.7345755859,2.0616271769\N,0.665667394,-2.3161551075,-1.0654570627\C,0.344854851,-3.6216071774,-0.5029640408\H,-0.4072790294,-3.5245252231,0.2827746293\H,-0.0701657404,-4.2595989236,-1.2875915853\H,1.2329429631,-4.1246124141,-0.0770242233\C,1.5640375095,-2.4818956872,-2.2000356715\H,1.1050462282,-3.1558223923,-2.9281121572\H,1.7369827354,-1.5230692506,-2.693616428\H,2.54208206,-2.9047164019,-1.9025853263\Version=ES64L-G09RevE.01\State=1-A\HF=-672.439557\RMSE=5.156e-09\RMSEF=5.634e-06\Dipole=-0.8839011,1.3333703,-0.294966\Quadrupole=-5.1685002,4.0425457,1.1259545,4.3189151,-5.7423147,4.6884626\PG=C01 [X(C12H17N1O2)]\@

3c(iv) [product]

1\1\GINC-R539\FOpt\RM062X\6-31+G(d,p)\C12H18N1O2(1+)\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdis sk=1610612736\la1\1,1\C,1.4825631395,0.9573511139,0.6286487864\C,0.6896944351,0.2039835788,1.744205151\C,1.4791821725,0.0273765714,-0.60512762\C,1.2381120164,-1.3724153934,-0.0314530345\C,0.2570641445,-1.14317903,1.1253060177\H,2.4076787659,0.1042208079,-1.176851786\H,0.6454589167,0.3020499561,-1.2662901305\H,2.1705731853,-1.829218453,0.3140601909\H,0.2656546629,-1.952162573,1.8611505918\H,-0.7625277176,-1.051464886,0.7258179915\C,2.906412868,1.2120870517,1.1754846476\C,1.631804694,0.018780038,2.9837748092\C,2.133387606,1.3801962827,3.4037398462\C,2.8047652725,2.0165653073,2.4447618183\H,3.5698766409,1.6462339547,0.4279253142\H,1.1470133708,-0.5501084619,3.7763387025\H,1.9508752935,1.7659385708,4.4001793866\H,3.2401560929,3.0048651819,2.5311722643\C,2.7976016607,-0.7756613065,2.4273946774\O,3.4670231248,-0.0960382599,1.4661765928\O,3.0526950147,-1.9275247394,2.6644159639\H,1.0295632828,1.9203664668,0.3858786688\H,-0.1808946179,0.7721781327,2.0754755476\N,0.698515831,-2.3463696554,-1.0558687527\H,-0.1853348647,-1.9611404953,-1.4077364348\C,0.4038115787,-3.68087712,-0.4414192202\H,-0.3731515857,-3.5660851593,0.3119421402\H,0.0710422095,-4.3628156653,-1.2234584824\H,1.3216618947,-4.0496111036,0.0195689227\C,1.6263290829,-2.4966211643,-2.221006592\H,1.2044309592,-3.221816685,-2.9163565445\H,1.7467383312,-1.5327060333,-2.7119976379\H,2.5867113839,-2.8509968303,-1.8434617961\Version=ES64L-G09RevE.01\State=1-A\HF=-672.8206767\RMSE=7.344e-09\RMSEF=8.444e-06\Dipole=-2.3759567,-0.9016773,-3.0360605\Quadrupole=-10.7765404,4.7064249,6.0701155,10.3283832,2.2096925,16.7605746\PG=C01 [X(C12H18N1O2)]\@

5e(ii) [product]

1\1\GINC-R3267\FOpt\RM062X\6-31+G(d,p)\C12H13O4(1-)\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdis k=2147483648\la6\1,1\C,1.5494846974,0.8623816681,0.5298871784\C,0.7443481619,0.0313774993,1.5737202797\C,1.5730729462,0.2174431932,-0.8591896249\C,2.0192739087,-1.2514409736,-0.9069654307\C,1.3990576969,-2.0840362877,0.2317311219\C,0.3109885767,-1.3343444011,1.0107748824\H,2.200358987,0.8000113568,-1.5414075077\H,0.5521108307,0.2836737493,-1.261394759\H,3.1117456914,-1.2759096945,-0.8275292051\H,2.1760873634,-2.4363783983,0.9177523347\H,-0.0692096107,-1.955506397,1.8334191829\H,-0.5358761823,-1.1645148466,0.3344990412\C,2.9404344747,1.1360712131,1.1479612376\C,1.6005183566,-0.0802500871,2.8803046966\C,1.9913768303,1.3210156813,3.3082478278\C,2.7143637704,1.9673606049,2.390990507\H,3.6299210638,1.5779686847,0.4278421925\H,1.0937438455,-0.6569845076,3.654422802\H,1.6943601184,1.7288589655,4.2691970375\H,3.070430892,2.9883991786,2.4784921031\C,2.9161269978,-0.7535254844,2.5369385093\O,3.564337081,-0.1125054786,1.5445536826\O,3.3852526147,-1.7248169042,3.0767467992\H,0.9433950283,-2.9667062714,-0.2274836611\H,1.0869645929,1.8517852445,0.425487542\H,-0.1558467389,0.5871121146,1.8621116572\C,1.6623317168,-1.76536952,-2.3484793583\O,0.7736035227,-2.6439480529,-2.4371004203\O,2.2936917659,-1.1848428488,-3.2633446484\Version=ES64L-G09RevE.01\State=1-A\HF=-765.786417\RMSE=6.081e-09\RMSEF=8.275e-06\Dipole=-0.4181166,3.6418785,5.0322041\Quadrupole=14.4412826,12.5040768,-26.9453594,-1.1845855,-9.295827,-11.6604279\PG=C01 [X(C12H13O4)]\@

5e(i) [product]

1\1\GINC-R185\FOpt\RM062X\6-31+G(d,p)\C12H14O4\ROOT\07-Aug-2017\0\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=214 7483648\|a4\|0,1\C,1.6148426678,0.8539322729,0.4966446268\C,0.75307461 48,0.100877771,1.5557713373\C,1.6636476321,0.1392625429,-0.8599461496\ C,2.0278722704,-1.3599351738,-0.775022393\C,1.1991772683,-2.1115399038 ,0.2896263865\C,0.181770987,-1.2154767992,1.0068336987\H,2.3696719889, 0.6510642898,-1.5219902107\H,0.673997277,0.2338049624,-1.324791245\H,3 .0952766119,-1.4352383316,-0.5474992269\H,1.8749237962,-2.5711105614,1 .0139447774\H,-0.2842160217,-1.7769305557,1.8244442455\H,-0.6268973539 , -0.9655954519,0.3094351659\C,3.0051663259,1.0946123742,1.1272978407\C ,1.6124445296,-0.0762955562,2.8528768914\C,2.0700505352,1.3010091736,3 .2902854437\C,2.8106317913,1.9251183758,2.3735783304\H,3.7151763584,1. 5191236284,0.4165577679\H,1.0785946624,-0.6339420866,3.6220953987\H,1. 8029886797,1.7075947458,4.2596193648\H,3.2208941636,2.9237842857,2.470 2801343\C,2.8812792026,-0.8210224653,2.4819047404\O,3.5683276145,-0.18 7663504,1.5019470475\O,3.2756242232,-1.8543018588,2.9543476976\H,0.657 6147788,-2.9284830956,-0.1942276145\H,1.1884025623,1.8465561956,0.3178 675082\H,-0.0895822295,0.7349323255,1.8488322552\C,1.8409931907,-1.948 8152691,-2.1572713776\O,0.9783124776,-2.7194318224,-2.5029471897\O,2.7 602287162,-1.4729419319,-3.0252997417\H,2.5700556788,-1.8669905763,-3. 8904605102\|Version=ES64L-G09RevE.01\|State=1-A\|HF=-766.341393\|RMSD=4.9 85e-09\|RMSF=5.957e-06\|Dipole=-0.6846547,1.9249773,-0.253994\|Quadrupole =-3.0982478,0.1182057,2.980042,0.7783377,-8.116802,3.023039\|PG=C01 [X(C12H14O4)]\|@

5e(iii) [product]

1\1\GINC-R2795\FOpt\RM062X\6-31+G(d,p)\C13H19N1O2\ROOT\07-Aug-2017\0\ #M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk= 2147483648\|a4\|0,1\C,1.7972682345,0.9953377479,0.585304833\C,0.718076 2619,0.4039406074,1.5436518632\C,1.7632877954,0.3735707145,-0.81682376 37\C,1.7944382195,-1.1591883002,-0.8493854353\C,0.8005762866,-1.781977 4634,0.1737342775\C,-0.0712615241,-0.7404072983,0.8869017353\H,2.59791 73781,0.7526332199,-1.4167393129\H,0.8494462334,0.7334638752,-1.302936 7665\H,2.8056064991,-1.4648891262,-0.5638837164\H,1.3472428607,-2.3820 060245,0.904943945\H,-0.6971452741,-1.2303767397,1.64221292\H,-0.76188 57324,-0.2955683711,0.1588189224\C,3.1588712197,0.8725698843,1.3061689 565\C,1.4187151259,-0.0071947457,2.8823554346\C,2.1457024684,1.2108035 069,3.4175513748\C,3.0748765669,1.6769880822,2.5821713451\H,3.99511611 15,1.1459710485,0.6617415624\H,0.7192778341,-0.4543327483,3.5885203274 \H,1.9100946229,1.6329223595,4.3884133113\H,3.6948330079,2.5492653921, 2.7553928839\C,2.5113392496,-1.0077702326,2.5558948477\O,3.384591546,- 0.5192808056,1.6452377727\O,2.632949994,-2.1153172011,3.0099894867\H,0 .1377394786,-2.4880480701,-0.3387838532\H,1.6231156361,2.0696479531,0. 4641493179\H,0.0067245105,1.190503397,1.8153199241\N,1.6353533045,-1.6 296816006,-2.233576774\C,2.0701496332,-3.0081117489,-2.3896463631\H,2. 0672595793,-3.2711714205,-3.4517246044\H,3.0894650279,-3.1198465122,-2 .0104354012\H,1.4224158141,-3.7317642475,-1.861073513\C,0.3087628683,- 1.4567000997,-2.8011105692\H,-0.0212545379,-0.4189129489,-2.7195002281 \H,0.3463480924,-1.7064347148,-3.8654972827\H,-0.4590203922,-2.1018813 687,-2.3360804579\|Version=ES64L-G09RevE.01\|State=1-A\|HF=-711.7290666\ RMSD=5.563e-09\|RMSF=6.420e-06\|Dipole=-0.8347899,1.5089484,-0.3322311\|Q uadrupole=0.4854751,1.2371495,-1.7226246,3.8732385,-2.120328,7.8495801 \|PG=C01 [X(C13H19N1O2)]\|@

5e(iv) [product]

1\1\GINC-R216\FOpt\RM062X\6-31+G(d,p)\C13H20N1O2(1+)\ROOT\07-Aug-2017\ 0\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdi sk=2147483648\|a6\|1,1\C,1.7171667992,0.9213485717,0.5482286003\C,0.73 57916046,0.3343793763,1.6027995624\C,1.7404021081,0.1204738436,-0.7790 949269\C,1.7159033403,-1.3984608491,-0.5759029732\C,0.4964821644,-1.85 95516356,0.2552962653\C,-0.2038074854,-0.7051920608,0.9897644925\H,2.6 322762893,0.4253967267,-1.3340724882\H,0.8665042289,0.4144836796,-1.37 71664614\H,2.6493268443,-1.7296734258,-0.114436511\H,0.8149859609,-2.6 247690566,0.9672192223\H,-0.8529035259,-1.1238988704,1.7641880932\H,-0 .8644826385,-0.1787753445,0.290934848\C,3.1165279907,0.9892181656,1.20

88765123\C,1.5811760854,-0.1639797276,2.8287040565\C,2.2429676844,1.07
13851084,3.4042911695\C,3.0282436185,1.7044827292,2.5335237633\H,3.874
2953113,1.3964675065,0.5389376911\H,0.9777905452,-0.7267721375,3.54059
27844\H,2.0541993637,1.389996766,4.4232427794\H,3.5725400014,2.6209634
699,2.7269316651\C,2.6804935692,-1.0531597866,2.2786713777\O,3.5161547
801,-0.3849423049,1.446390902\O,2.8025767034,-2.2396257601,2.440873172
2\H,-0.249922604,-2.3275356722,-0.4007454784\H,1.4235922411,1.94375649
08,0.2942467071\H,0.1117586233,1.1419864275,1.9934453802\N,1.710621673
7,-2.1415003179,-1.9129696534\H,0.7904242065,-1.9913319189,-2.34113357
6\C,2.7467200979,-1.6546331459,-2.8763695803\H,2.7703632211,-2.3301443
729,-3.731134366\H,2.4985815918,-0.6490282978,-3.2082142052\H,3.712508
231,-1.6613919834,-2.3682047182\C,1.8801048515,-3.6158135532,-1.694561
0242\H,1.1168439349,-3.9758749982,-1.0084355381\H,1.7954272,-4.1258722
808,-2.6536914602\H,2.8700513877,-3.776450361,-1.2650840842\Version=E
S64L-G09RevE.01\State=1-A\HF=-712.1142186\RMSD=4.218e-09\RMSF=8.693e-0
6\Dipole=-1.0957507,-0.3765223,-3.6255424\Quadrupole=-11.5776488,-1.18
01891,12.7578379,4.6812371,-3.0439335,18.0005142\PG=C01 [X(C13H20N1O2)
]\@

3d(ii) [product]

1\1\GINC-R544\FOpt\RM062X\6-31+G(d,p)\C11H11O4(1-)\ROOT\07-Aug-2017\O\
#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk
=1610612736\|a5\|1,\C,1.2882564117,0.9585139611,0.5050087677\C,0.453
6105836,0.20323556,1.5910924556\C,1.3380751703,0.017202681,-0.71105198
98\C,1.1457810028,-1.3768855191,-0.1061726492\C,0.0462244074,-1.127142
0723,0.933453236\C,0.6135046647,2.3236326031,0.2778713375\C,-0.7146250
546,1.1276826435,2.0512143313\C,-0.1100444681,2.432203912,2.5333598352
\C,0.5975927677,3.0664826581,1.596013594\H,2.2621423837,0.1094359225,-
1.2864899229\H,0.506053868,0.2167386396,-1.3965926137\H,2.0662548474,-
1.6624244543,0.4303685422\H,-0.0579319802,-1.9498639445,1.6437247756\H
,-0.9155450878,-1.0274422171,0.4106944457\H,-0.2507232383,2.7862540443
,3.5497290392\H,1.1334838357,3.9985139412,1.7411608724\H,1.0580916581,
2.8845643319,-0.5450944136\H,-1.3736784832,0.6436787777,2.771955885\C,
-1.514689115,1.481044911,0.8085357948\O,-0.7594580204,2.0902843392,-0.
1309266591\O,-2.6885156405,1.2746627277,0.6315428905\H,2.301304584,1.1
541413714,0.8754091593\H,1.0745318109,0.0095274339,2.4730043682\C,0.84
76660144,-2.5254904589,-1.1124292101\O,1.1785839258,-2.3052276812,-2.3
004365607\O,0.3363531521,-3.5495731121,-0.6016073109\Version=ES64L-GO
9RevE.01\State=1-A\HF=-726.4932983\RMSD=7.482e-09\RMSF=3.896e-06\Dipol
e=0.8819304,5.1153164,3.7164017\Quadrupole=9.9598827,-16.847228,6.8873
453,9.7884843,3.9554686,-17.7656956\PG=C01 [X(C11H11O4)]\@

3d(i) [product]

1\1\GINC-R828\FOpt\RM062X\6-31+G(d,p)\C11H12O4\ROOT\07-Aug-2017\O\
#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=161
0612736\|a1\|O,1,\C,1.3269304389,0.9320939323,0.5608882814\C,0.41164504
97,0.2018191907,1.5960195364\C,1.380864346,0.0197707901,-0.6765466446\
C,1.0790985711,-1.3709586073,-0.1167871183\C,-0.0368836501,-1.10290804
4,0.9123608104\C,0.7125605322,2.3225375914,0.3080909648\C,-0.750446794
1,1.1594130537,1.9958149952\C,-0.1360452034,2.4422899281,2.5179439906\
C,0.6432936165,3.0570732351,1.6275384178\H,2.3378387333,0.0708998805,-
1.2011113904\H,0.5946759734,0.2893637824,-1.3900782161\H,1.9537279406,
-1.7759232706,0.4105312091\H,-0.1741122988,-1.9277278843,1.6146489677\
H,-0.987031136,-0.9557509873,0.3821358351\H,-0.336627456,2.8009750386,
3.5215267209\H,1.1866729735,3.9787273435,1.8014683472\H,1.2234985257,2
.8740120086,-0.481337455\H,-1.4619925961,0.6911610024,2.6754529845\C,-
1.4590425088,1.5127614271,0.6971355179\O,-0.6338642037,2.1178506128,-0
.1876446264\O,-2.6039039896,1.2692563742,0.4227359247\H,2.3294989985,1
.0764457491,0.9749267734\H,0.9764564694,-0.0284848419,2.5042735289\C,0
.6852582999,-2.3783577087,-1.1654472688\O,0.6056759647,-2.1721471173,-
2.3511200235\O,0.4104702571,-3.5822562222,-0.6198563267\H,0.1519131463
,-4.175466257,-1.342163736\Version=ES64L-G09RevE.01\State=1-A\HF=-727
.0470347\RMSD=8.623e-09\RMSF=1.570e-05\Dipole=1.6944919,-0.1060243,1.4
690766\Quadrupole=-5.7826468,7.4363845,-1.6537377,5.8406833,-1.3473295
,2.4502704\PG=C01 [X(C11H12O4)]\@

3d(iii) [product]

1\1\GINC-R154\FOpt\RM062X\6-31+G(d,p)\C12H17N1O2\ROOT\07-Aug-2017\0\#\#
M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=1
610612736\|a1\|0,1\C,1.3475059427,0.9800000506,0.5311132788\C,0.530522
2033,0.2354683145,1.6320406041\C,1.4629638546,-0.0043230868,-0.6431188
721\C,1.3077220228,-1.3904935425,-0.0003615153\C,0.2070141459,-1.14742
00928,1.0424338338\C,0.5949922288,2.2850015949,0.2042685262\C,-0.71577
63226,1.0978293294,1.9956212802\C,-0.2229738634,2.4659705956,2.4210088
598\C,0.4771122689,3.0940545687,1.4755197555\H,2.4035070877,0.12274756
89,-1.1853667746\H,0.6329987052,0.1350430695,-1.3470319727\H,2.2524457
931,-1.6458660896,0.531228187\H,0.1624018562,-1.9157989613,1.818522099
9\H,-0.7582404629,-1.1407018738,0.517722743\H,-0.4384906194,2.86742507
66,3.4052047676\H,0.9322674409,4.0724382697,1.5788439492\H,1.035980330
5,2.8307709055,-0.6302075751\H,-1.3654156179,0.6074190204,2.7201395563
\C,-1.4797797989,1.2973248432,0.6961299639\O,-0.7332215499,1.920253409
7,-0.2454444741\O,-2.6030362947,0.9353202526,0.4670785427\H,2.33971479
29,1.2488394823,0.9059399475\H,1.1294196349,0.1288737501,2.5412174178\
N,0.9763006851,-2.4366746524,-0.9566309998\C,0.7469471224,-3.711847193
8,-0.2949766429\H,-0.1114540507,-3.6451201772,0.3762312475\H,0.5251023
48,-4.4735655983,-1.0465557129\H,1.6264203343,-4.0467563465,0.28882670
05\C,2.0101934667,-2.5792479588,-1.9698993987\H,1.7358778267,-3.385481
6654,-2.6547858209\H,2.1020207637,-1.6614066472,-2.5539684288\H,2.9986
377252,-2.8183262158,-1.5313230733\Version=ES64L-G09RevE.01\State=1-A
\HF=-672.4385184\RMSE=6.546e-09\RMSEF=1.423e-05\Dipole=1.9077686,0.0391
946,0.8461114\Quadrupole=-9.2558283,5.8765167,3.3793115,3.5474025,-4.1
586576,2.4900581\PG=C01 [X(C12H17N1O2)]\@

3d(iv) [product]

1\1\GINC-R160\FOpt\RM062X\6-31+G(d,p)\C12H18N1O2(1+)\ROOT\07-Aug-2017\
0\#\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdi
sk=1610612736\|a1\|1,1\C,1.4345441754,1.0082343073,0.6195538863\C,0.59
4900595,0.2748949544,1.7119997851\C,1.6005005547,0.0097231899,-0.54305
06301\C,1.399987332,-1.3710327175,0.0906384636\C,0.3718613123,-1.16726
83071,1.2109381238\C,0.6528821694,2.276968924,0.2020688212\C,-0.739398
755,1.0651928588,1.9155234634\C,-0.3755784282,2.4746634707,2.324669487
4\C,0.3768169366,3.1112242528,1.4280359728\H,2.5659686463,0.1143867778
,-1.0427690858\H,0.8080184554,0.1887651463,-1.2831040181\H,2.341586922
, -1.7805438104,0.473928285\H,0.4735172179,-1.8990715575,2.0151501558\H
, -0.6439164952,-1.2651309658,0.800493869\H,-0.714526406,2.8941396514,3
.2649520344\H,0.7547831867,4.1215383177,1.5282510759\H,1.1365344806,2.
8242632646,-0.6067513181\H,-1.4187731614,0.5551596629,2.5979572482\C,-
1.3518768032,1.1023942042,0.5242031029\O,-0.601278025,1.8070440021,-0.
3530318509\O,-2.3229197024,0.4907514467,0.1629488695\H,2.4082258929,1.
3080693574,1.0139149748\H,1.1260500169,0.2702179581,2.6658921122\N,0.9
116689766,-2.3858380749,-0.9253450692\H,0.0202526093,-2.0212841015,-1.
2854029663\C,0.6376898076,-3.7199195653,-0.304502834\H,-0.1235853858,-
3.610520718,0.4655147001\H,0.2895788327,-4.4031228012,-1.078765408\H,1
.56794834,-4.0887726665,0.1302656835\C,1.8483259493,-2.5264959256,-2.0
836323649\H,1.4466911357,-3.2691689629,-2.7725589364\H,1.947622695,-1.
5665016116,-2.5864695524\H,2.8151869221,-2.8557699615,-1.6998560808\Ver
sion=ES64L-G09RevE.01\State=1-A\HF=-672.81785\RMSE=7.815e-09\RMSEF=6.
324e-06\Dipole=2.5874289,-3.122782,-0.7445944\Quadrupole=-16.0265064,1
7.3574314,-1.330925,-2.8836832,-7.5191509,13.6749434\PG=C01 [X(C12H18N
1O2)]\@

5g(ii) [product]

1\1\GINC-R805\FOpt\RM062X\6-31+G(d,p)\C12H13O4(1-)\ROOT\07-Aug-2017\0\
\#\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk
=2147483648\|a1\|-1,1\C,1.2962286568,0.9414005632,0.3720768096\C,0.501
4732785,0.1210119813,1.4355174403\C,1.4407041051,0.1958136004,-0.95591
5207\C,1.9947865227,-1.2121660276,-0.7101828106\C,1.0657120941,-2.0255
95831,0.2143707012\C,-0.0499732154,-1.1783767972,0.8412415416\C,0.5964
633501,2.310695537,0.2429262435\C,-0.6311388187,1.0308185416,2.0166270
077\C,-0.0071662174,2.3095775725,2.5311138152\C,0.643179992,2.99426536
57,1.5879745332\H,2.1299359002,0.7254818363,-1.620226709\H,0.472954943
5,0.1399751953,-1.4713037276\H,2.9744094108,-1.0786579595,-0.227468322
6\H,1.6506020832,-2.4930193228,1.0180863404\H,-0.5743523174,-1.7429290
573,1.6233216011\H,-0.8038500139,-0.9403737396,0.0799809721\H,-0.08973

7241,2.6074371935,3.5714842161\H,1.1892596336,3.9177544935,1.748204104
1\H,1.0017988925,2.9039609555,-0.5772359224\H,-1.2453566433,0.50445065
18,2.7476438513\C,-1.4970589484,1.4284694179,0.8344015933\O,-0.7936565
653,2.0804537452,-0.1132158417\O,-2.6750649594,1.2056781591,0.70288820
79\H,0.6401163911,-2.8377942186,-0.3830968139\H,2.3066836308,1.1394452
748,0.7508279495\H,1.1644591714,-0.1346438731,2.2713777379\C,2.3130611
889,-1.9021211832,-2.0887930291\O,3.1038802531,-1.2461809591,-2.807390
7297\O,1.7600254419,-3.0004311157,-2.3179055524\Version=ES64L-G09RevE
.01\State=1-A\HF=-765.7930878\RMSD=6.668e-09\RMSF=6.266e-06\Dipole=-1.
1026481,3.657407,4.9006506\Quadrupole=-2.7761518,2.548574,0.2275778,17
.6509957,18.3890295,-20.1451502\PG=C01 [X(C12H13O4)]\@

5g(i) [product]

1\1\GINC-R261\FOpt\RM062X\6-31+G(d,p)\C12H14O4\ROOT\07-Aug-2017\0\#M0
62X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=214
7483648\|a3\|0,1\C,1.33935841,0.9441004661,0.4115984308\C,0.5176208855
.0.1265323807,1.4570721983\C,1.4352173123,0.2343485653,-0.9407893446\C
.2.0024143175,-1.1917784163,-0.7724632103\C,1.2759221488,-1.9881168557
.0.3350366726\C,0.0741152464,-1.2283823751,0.9005809061\C,0.6548508521
.2.3226583243,0.2710317802\C,-0.6844491654,1.0037426011,1.9326141713\C
,-0.124215557,2.2870376046,2.503958412\C,0.5982421642,2.9835668952,1.6
258486184\H,2.0769461994,0.8058076719,-1.6181326472\H,0.4430160948,0.1
886524448,-1.4040038232\H,3.0691096214,-1.0941996988,-0.5349830332\H,1
.9781444854,-2.1923521885,1.1512557747\H,-0.3952632339,-1.8142817704,1
.6978847672\H,-0.6903676194,-1.0973546203,0.1246817659\H,-0.30525067,2
.578514543,3.5328583834\H,1.1079962936,3.9177575485,1.8317461247\H,1.1
165040133,2.9371898159,-0.5026046448\H,-1.3432881522,0.4588621135,2.60
84711591\C,-1.454037924,1.374334899,0.6754799032\O,-0.69447492,2.07886
61704,-0.196548216\O,-2.588932195,1.074195875,0.4171377346\H,0.955592
986,-2.9528811338,-0.0652694146\H,2.3547084405,1.1152094651,0.78816964
26\H,1.1412788778,-0.0567151093,2.3395513239\C,1.9381977883,-1.8956866
032,-2.112662013\O,1.2720876357,-2.8637008784,-2.3855175545\O,2.724342
324,-1.2868874315,-3.0265511969\H,2.6187360272,-1.7660843031,-3.862804
6707\Version=ES64L-G09RevE.01\State=1-A\HF=-766.3445336\RMSD=5.921e-0
9\RMSF=3.869e-06\Dipole=2.0195907,0.500859,0.9096136\Quadrupole=-8.140
9228,-0.9636728,9.1045957,2.9055274,-3.7362175,0.2823154\PG=C01 [X(C12
H14O4)]\@

5g(iii) [product]

1\1\GINC-R1172\FOpt\RM062X\6-31+G(d,p)\C13H19N1O2\ROOT\07-Aug-2017\0\|
#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=
2147483648\|a4\|0,1\C,1.3576682753,0.9567875166,0.4163739411\C,0.60015
14956,0.1263774456,1.5002957187\C,1.581516054,0.1646360588,-0.87499802
57\C,2.3148344873,-1.1596045946,-0.6265309427\C,1.7412664752,-1.905293
0233,0.6140970986\C,0.3990756713,-1.3280904027,1.0673480108\C,0.513805
8312,2.2245251884,0.1466844454\C,-0.7394236093,0.8567036726,1.83539692
82\C,-0.3900731032,2.2416736628,2.3322034564\C,0.2917009894,2.96400686
37,1.4424763881\H,2.1633310571,0.7584604812,-1.5875795246\H,0.61086790
51,-0.0193096578,-1.3451153554\H,3.3633376704,-0.9106464046,-0.4186872
535\H,2.4492070596,-1.831193524,1.449071635\H,-0.0072448695,-1.9054479
961,1.9051815318\H,-0.339833346,-1.3932021897,0.2577072393\H,-0.670428
1322,2.577469012,3.3247352337\H,0.6632298196,3.9697245518,1.6023471954
\H,0.9361422802,2.8396778833,-0.6484400524\H,-1.3609894013,0.275844928
7,2.5167392512\C,-1.468048613,1.0226500698,0.5121911021\O,-0.766946254
8,1.7767091967,-0.3647294636\O,-2.5257164467,0.5335383975,0.2132637272
\H,1.6436089841,-2.9742068008,0.3961310526\H,2.3277593614,1.2822361834
,0.8104240673\H,1.1905850599,0.1212503643,2.4237348465\N,2.3518191663,
-1.9516830999,-1.8622108932\C,3.3885901759,-2.9686244309,-1.8340014905
\H,4.3539089983,-2.5081425352,-1.6050510707\H,3.1997405025,-3.76776922
4,-1.0929160741\H,3.459878811,-3.4396340277,-2.818807293\C,1.078409843
4,-2.5409968209,-2.2467043634\H,1.1812374547,-2.9827925875,-3.24187418
88\H,0.7399354915,-3.3385649208,-1.5605145284\H,0.2954588557,-1.782055
2367,-2.3023503495\Version=ES64L-G09RevE.01\State=1-A\HF=-711.733338\
RMSD=3.385e-09\RMSF=2.656e-06\Dipole=1.6404547,0.0612744,1.025866\Quad
rupole=-9.7592508,6.5970931,3.1621578,2.1727546,-2.1033328,3.3311783\PG
G=C01 [X(C13H19N1O2)]\@

5g(iv) [product]

1\1\GINC-R259\FOpt\RM062X\6-31+G(d,p)\C13H20N1O2(1+)\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=2147483648\|a1\1,1\C,1.5218316026,0.8795359255,0.6299941015\C,0.460889811,0.0723898332,1.4428454825\C,1.8605504524,0.2255111356,-0.7216698017\C,2.2991080282,-1.2327983837,-0.5759824598\C,1.5351039857,-1.9860891297,0.5246547405\C,0.1991199213,-1.3184906562,0.855395846\C,0.9220543955,2.2874901664,0.3671829078\C,-0.8413769187,0.9331391324,1.5332624417\C,-0.4849726431,2.2062947515,2.2647537574\C,0.4749560309,2.9092394308,1.6648186334\H,2.6417765654,0.8118276013,-1.2157656959\H,0.9684572429,0.2900625237,-1.3532713994\H,3.3753864097,-1.2848056095,-0.3805208526\H,2.1604524023,-1.97918551,1.424067794\H,-0.3497831702,-1.9239382522,1.5820231368\H,-0.4432434889,-1.2434298622,-0.0311532792\H,-0.9740209763,2.4821267614,3.192174309\H,0.8947354177,3.8399950651,2.0269872035\H,1.5902220241,2.9216623936,-0.2162697548\H,-1.6671046049,0.372898377,1.9714822339\C,-1.1727409928,1.2744922712,0.08907845\O,-0.2306236131,2.0660071971,-0.4812741157\O,-2.0909444629,0.8408369716,-0.5534449137\H,1.4132999504,-3.0448939312,0.2640774295\H,2.4383905348,0.9994071565,1.2168949844\H,0.8268579391,-0.0554519807,2.4664846586\N,2.1607529734,-1.9675235938,-1.9185812437\H,2.5749708031,-2.8910253787,-1.7577329086\C,0.7531118379,-2.2116748171,-2.3750430075\H,0.2198103817,-2.7844353989,-1.6189992058\H,0.2564585355,-1.2571682744,-2.5457947859\H,0.7943710074,-2.7757569745,-3.3069743943\C,2.9585891138,-1.315098597,-3.0034874639\H,2.9930936224,-1.9840402531,-3.8633123218\H,2.4704141138,-0.3816961854,-3.2817127988\H,3.9666457679,-1.1203539055,-2.6364477075\Version=ES64L-G09RevE.01\State=1-A\HF=-712.1130252\RMSD=7.754e-09\RMSE=2.772e-05\Dipole=3.4062531,-2.9099032,-1.2916864\Quadrupole=-10.5909184,5.5247803,5.0661381,-5.4713617,-14.0949239,16.2855236\PG=C01 [X(C13H20N1O2)]\|@

5f(ii) [product]

1\1\GINC-R270\FOpt\RM062X\6-31+G(d,p)\C12H13O4(1-)\ROOT\08-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=2147483648\|a5\1,1\C,1.5804611096,0.8474412969,0.5015154708\C,0.7642055523,0.0213741631,1.5383908636\C,1.5813956603,0.208574783,-0.8885871649\C,2.0332834462,-1.2588654518,-0.9461486485\C,1.4510307202,-2.1024014684,0.205916062\C,0.3632729789,-1.3657659604,0.9991680117\H,2.1941930155,0.793324696,-1.5811524273\H,0.5521715791,0.274124283,-1.2703811062\H,3.1287087938,-1.278990554,-0.9051527682\H,2.2439855822,-2.4347619952,0.8825746113\H,0.0107851257,-1.985107633,1.8360098883\H,-0.498831413,-1.2263125993,0.3352375514\C,3.0002670013,1.1159821215,1.111943352\C,1.6020587719,-0.0459606171,2.8357376325\C,1.9859183951,1.355207073,3.2552010258\C,2.7560069997,1.9602861043,2.3482536511\H,3.67930364,1.563002092,0.3859211685\H,1.1009095331,-0.6208163847,3.6164736015\H,1.6496442514,1.7960789037,4.1875551107\H,3.151143231,2.9673571713,2.4382899424\O,2.8200558523,-0.7755443042,2.55650895\C,3.6044207638,-0.1794985794,1.6289037463\O,4.6722374724,-0.6470630041,1.3273404472\H,0.9999126262,-2.9890979677,-0.2496634781\H,1.1294834138,1.8429227441,0.4095126329\H,-0.1519809805,0.5661505616,1.7992663557\C,1.6379038398,-1.7756734066,-2.3805510145\O,2.2113140588,-1.1656717006,-3.3130974824\O,0.7798929788,-2.6860433669,-2.4415529855\Version=ES64L-G09RevE.01\State=1-A\HF=-765.7855353\RMSD=5.651e-09\RMSE=9.959e-06\Dipole=-0.6109507,3.3567654,5.4166379\Quadrupole=9.4707005,12.081047,-21.5517474,-2.8159054,-9.3058156,-14.2342567\PG=C01 [X(C12H13O4)]\|@

5f(i) [product]

1\1\GINC-R281\FOpt\RM062X\6-31+G(d,p)\C12H14O4\ROOT\08-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=2147483648\|a3\0,1\C,1.5578949661,0.8631451197,0.497699092\C,0.7576824125,0.0303443011,1.5434428882\C,1.5632308295,0.2216234438,-0.8934023758\C,2.0337989084,-1.2514062141,-0.9127573429\C,1.397757697,-2.1023514324,0.2085365106\C,0.3233862242,-1.3414170949,0.9961568038\H,2.1859257126,0.8118018415,-1.5727013841\H,0.5384984009,0.2721862121,-1.2841762994\H,3.1253843299,-1.2605979453,-0.8245306011\H,2.181181441,-2.4519156447,0.8832960033\H,-0.0324861636,-1.9648062118,1.8246261252\H,-0.5426141802,-1.1830293294,0.3421798287\C,2.9808909898,1.1499008697,1.0872264177\C,1.6312889431,-0.0642908377,2.8163215953\C,2.0179004779,1.3274540633

,3.2576827238\C,2.7570812443,1.9621668855,2.3472786638\H,3.6401276565,
1.6227390059,0.3592004877\H,1.1563348269,-0.6609037944,3.5956567166\H,
1.7105529356,1.7368058418,4.2131386311\H,3.1561017032,2.9650494692,2.4
538731327\O,2.8396744554,-0.7858096312,2.4727711984\C,3.5900172743,-0.
1683934794,1.5353080702\O,4.6082132425,-0.6627480721,1.1250481819\H,0.
9364531825,-2.9860771123,-0.2393461612\H,1.0902732513,1.8468193816,0.3
898252884\H,-0.1457713157,0.578604987,1.831249094\C,1.7199338845,-1.80
29522191,-2.2877525997\O,0.9003032397,-2.6480439434,-2.5554923843\O,2.
4581843497,-1.198064874,-3.2428250986\H,2.19468008,-1.5782975859,-4.09
47842062\Version=ES64L-G09RevE.01\State=1-A\HF=-766.3412013\RMSD=9.19
2e-09\RMSF=7.174e-06\Dipole=-1.1642348,1.5463006,0.3175751\Quadrupole=
-7.5519576,0.6360363,6.9159213,-0.0292905,-6.2642793,0.4848729\PG=C01
[X(C12H14O4)]\@

5f(iii) [product]

1\1\GINC-R295\FOpt\RM062X\6-31+G(d,p)\C13H19N1O2\ROOT\08-Aug-2017\O\#
M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=2
147483648\A2\O,1\C,1.627580811,0.83100465,0.5145736117\C,0.730139532
2,0.0848718341,1.5469343596\C,1.6303015178,0.1588963458,-0.8623141017\
C,2.0037933298,-1.3289546653,-0.8593063968\C,1.3063558818,-2.107882994
2,0.2940890427\C,0.2404101572,-1.2781536891,1.0221622453\H,2.310372993
2,0.6869790565,-1.5388940893\H,0.6242024915,0.2865492791,-1.2784554522
\H,3.0855483163,-1.3882803567,-0.7009623608\H,2.0531876672,-2.46530634
98,1.0061009417\H,-0.1822938575,-1.8557231393,1.8532461394\H,-0.590151
882,-1.08858971,0.3298760075\C,3.0436015746,1.0309620845,1.1580456405\
C,1.5359657823,-0.019423231,2.8632245089\C,2.0006313156,1.3579005621,3
.2738473525\C,2.8256677299,1.9028000669,2.3789516267\H,3.7659394933,1.
4282549856,0.4449911808\H,0.9853801948,-0.5511266514,3.6399965521\H,1.
6810725385,1.8238884673,4.1989053268\H,3.2913638324,2.8781488468,2.470
4209117\O,2.7051681018,-0.8346137439,2.6051133854\C,3.5360672165,-0.30
88225975,1.6785812079\O,4.5322957822,-0.8902686792,1.3337002643\H,0.82
6035682,-3.0053886829,-0.111424381\H,1.2393409133,1.844657812,0.374645
681\H,-0.1508279462,0.6951736439,1.7740549598\N,1.794750337,-1.8902438
311,-2.202440431\C,2.53440568,-3.1267044091,-2.3961385838\H,3.58888145
87,-2.968535515,-2.1553181729\H,2.1579778213,-3.9610695794,-1.77565827
26\H,2.4618035566,-3.4315221305,-3.4445112509\C,0.4056284335,-2.072107
2401,-2.5881369292\H,0.3673293047,-2.3509863549,-3.6452502268\H,-0.111
4199375,-2.8648457534,-2.0167583167\H,-0.1591828235,-1.1443173309,-2.4
729519805\Version=ES64L-G09RevE.01\State=1-A\HF=-711.7288202\RMSD=4.5
76e-09\RMSF=5.458e-06\Dipole=-1.5352141,0.9533783,0.190337\Quadrupole=
-5.2172676,4.375516,0.8417517,3.0323176,-3.3435649,4.6708763\PG=C01 [X
(C13H19N1O2)]\@

5f(iv) [product]

1\1\GINC-R320\FOpt\RM062X\6-31+G(d,p)\C13H20N1O2(1+)\ROOT\08-Aug-2017\
O\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdi
sk=2147483648\A6\1,1\C,1.2228454292,0.853215518,0.5953895139\C,0.854
1779535,-0.1401095544,1.7328330801\C,1.2505244793,0.1831128596,-0.8034
511846\C,1.8870382532,-1.2133918093,-0.806307899\C,1.2066373196,-2.179
9075177,0.1852515644\C,0.2982547794,-1.457755985,1.19017271\H,1.789214
4492,0.8538059083,-1.4788402913\H,0.2187454762,0.1044790741,-1.1731797
376\H,2.9545249332,-1.147435712,-0.5952775419\H,1.9782243159,-2.746819
3321,0.7127689479\H,0.0760865716,-2.1370100315,2.0185896495\H,-0.66403
55167,-1.2379381553,0.7133147532\C,2.5916330849,1.5361473611,0.9493682
361\C,2.1076734954,-0.2634566607,2.6341092178\C,2.3245946169,1.0864479
116,3.271524496\C,2.5525453945,2.0454051699,2.3745029132\H,2.873745036
1,2.2887272937,0.2135012261\H,2.0418481555,-1.088219079,3.3436657678\H
,2.2561568076,1.2311759226,4.3432506619\H,2.7283732986,3.0897267878,2.
6050914707\O,3.2473823564,-0.5845028369,1.7858080858\C,3.5906340798,0.
4015555696,0.9273328126\O,4.5165896551,0.2724776304,0.1663243691\H,0.5
871390389,-2.9095346186,-0.3534834699\H,0.4780488163,1.6512209044,0.54
55889746\H,0.0739090416,0.3017058235,2.357877256\H,1.875981265,-1.8190
063165,-2.2097570503\H,0.9015882119,-2.0359765331,-2.446617484\C,2.411
8697849,-0.8901509917,-3.2562218426\H,1.7114980031,-0.0741683759,-3.41
87756499\H,3.3717990871,-0.5054953456,-2.9050489076\H,2.5460761416,-1.
4505956572,-4.1809722431\C,2.6545565156,-3.1001688337,-2.2374036033\H,
2.5637206368,-3.5459218411,-3.2274689412\H,3.6973388213,-2.8577230711,

-2.0261293286\H,2.2694122115,-3.7822564763,-1.4828055319\\Version=ES64
L-G09RevE.01\State=1-A\HF=-712.1141158\RMSD=9.222e-09\RMSF=8.791e-06\D
ipole=-1.9397644,-1.4348812,-2.6385458\Quadrupole=-18.2872652,1.465128
7,16.8221364,0.4728399,-0.6221994,13.6957434\PG=C01 [X(C13H20N1O2)]\@

5h(ii) [product]

1\1\GINC-R328\FOpt\RM062X\6-31+G(d,p)\C12H13O4(1-)\ROOT\08-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk
=2147483648\|a3\|0,1\,C,1.2621464703,0.9375189037,0.2974560514\,C,0.560
3815344,0.0960645392,1.4085614573\,C,1.3847312232,0.1697280663,-1.01964
1833\,C,2.0191949813,-1.2019433899,-0.7624651596\,C,1.1538671257,-2.0473
439282,0.1936403292\,C,0.0367599468,-1.2377980064,0.8669214102\,C,0.5048
850288,2.3015788511,0.1667667489\,C,-0.5664548623,0.9689745641,2.002055
8978\,C,0.0197501656,2.2688570024,2.4975063759\,C,0.5742712782,2.9831628
604,1.5158415468\,H,2.015942099,0.7161464002,-1.7263241573\,H,0.40049004
55,0.0498756705,-1.4948287868\,H,2.9983710637,-1.0049954446,-0.30079021
23\,H,1.7865132544,-2.4993873008,0.9692880873\,H,-0.4147922234,-1.810036
9459,1.6887767303\,H,-0.7677494717,-1.0415379798,0.149614908\,H,-0.00328
02402,2.5523848211,3.5442401064\,H,1.0593972325,3.9455507883,1.64461309
36\,H,0.8854473902,2.8976189891,-0.6623977815\,H,-1.1549262991,0.4339467
616,2.7492785796\,O,-1.5008560437,1.2624245765,0.9318085123\,C,-0.959945
9617,1.9856911765,-0.0756714208\,O,-1.620393211,2.3169993236,-1.0272218
69\,H,0.7323265944,-2.8709725704,-0.3908018921\,H,2.277756537,1.18634120
43,0.6280748027\,H,1.2720735911,-0.1136094122,2.2175002618\,C,2.35299353
82,-1.9019072995,-2.1326922773\,O,1.8473679113,-3.0282793933,-2.3341697
953\,O,3.1057413013,-1.2250858283,-2.8717547145\\Version=ES64L-G09RevE.
01\State=1-A\HF=-765.7923693\RMSD=5.188e-09\RMSF=4.747e-06\Dipole=-1.4
202342,3.3684097,5.2878396\Quadrupole=1.2845283,-1.2119425,-0.0725858,
18.9617407,14.563682,-17.6653436\PG=C01 [X(C12H13O4)]\@

5h(i) [product]

1\1\GINC-R345\FOpt\RM062X\6-31+G(d,p)\C12H14O4\ROOT\08-Aug-2017\0\#M0
62X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=214
7483648\|a3\|0,1\,C,1.304719924,0.9264317907,0.3408557535\,C,0.561800928
1,0.0917340702,1.4308101026\,C,1.3736313247,0.1957088113,-1.0022725551\
C,1.9966220395,-1.2046368919,-0.8224189077\,C,1.2876201807,-2.026363340
3,0.2784881289\,C,0.1108448345,-1.2715274338,0.9018701661\,C,0.585582900
8,2.3070650098,0.2012794232\,C,-0.6202424056,0.9497054351,1.9326290613\
C,-0.0781178599,2.2449496524,2.4846219238\,C,0.5590275492,2.9665662006,
1.5618430205\,H,1.969311433,0.7764445995,-1.7126093757\,H,0.3704581595,0.
.0991361321,-1.4367227363\,H,3.0540495286,-1.0572568858,-0.5693280616\,H
,2.0092688748,-2.2711447949,1.0658730201\,H,-0.3102320019,-1.8606262447
,1.7240184823\,H,-0.6919201646,-1.141407175,0.1678631211\,H,-0.196425387
5,2.5211627027,3.5261530629\,H,1.0229697635,3.9314574424,1.7348871054\,H
,1.0250538629,2.9181977696,-0.5868898855\,H,-1.2611068292,0.4049898868,
2.6266814615\,O,-1.4615478073,1.2345968916,0.7874911751\,C,-0.8543532064
,1.9821907471,-0.1623794118\,O,-1.4214038842,2.291566212,-1.1764253682\
H,0.9409024694,-2.9715408605,-0.1462094023\,H,2.3290967622,1.1323162028
,0.6718381387\,H,1.2310139669,-0.0733752239,2.2834331129\,C,1.9853921878
, -1.915761875,-2.1605095705\,O,1.3499196031,-2.900740841,-2.4457329611\
O,2.7803500862,-1.2917876202,-3.0556216015\,H,2.705575167,-1.7730563697
, -3.8939943228\\Version=ES64L-G09RevE.01\State=1-A\HF=-766.3444638\RMS
D=7.445e-09\RMSF=1.037e-05\Dipole=1.6514558,0.1324455,1.3829587\Quadru
pole=-4.4008493,-3.4872115,7.8880608,4.1170601,-5.9865652,1.9751812\PG
=C01 [X(C12H14O4)]\@

5h(iii) [product]

1\1\GINC-R364\FOpt\RM062X\6-31+G(d,p)\C13H19N1O2\ROOT\08-Aug-2017\0\#
M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=2
147483648\|a5\|0,1\,C,1.1765065432,0.8845422455,0.2299194297\,C,0.658964
4959,0.1001624891,1.4770962266\,C,1.2122025392,0.0088019276,-1.02557153
66\,C,2.0460498002,-1.2616948803,-0.776690973\,C,1.5303339339,-2.0320695
,0.4690193408\,C,0.3330620824,-1.35798631,1.142720471\,C,0.2713184445,2.
1439093054,0.0317712505\,C,-0.5662994313,0.8663563625,2.0210243562\,C,-0
.1453025152,2.2725479299,2.3699277753\,C,0.2942986478,2.9515563685,1.30
9772909\,H,1.6365581036,0.583821393,-1.8569799376\,H,0.1907199871,-0.259

3165335,-1.3223253271\H,3.0727236842,-0.9312540947,-0.569611843\H,2.34
45317394,-2.1207490194,1.1976458207\H,0.0690900834,-1.8925864304,2.062
3378016\H,-0.5490848074,-1.398987701,0.4932560395\H,-0.1925704809,2.65
28710293,3.3839616417\H,0.6430771688,3.978398453,1.3278103518\H,0.5458
447221,2.7056015907,-0.8609223435\H,-1.0579720457,0.3351478764,2.83674
15586\O,-1.5497180158,0.914075598,0.9567326431\C,-1.1417919118,1.60847
09954,-0.1302222094\O,-1.842778853,1.7233254016,-1.1007803237\H,1.2789
984037,-3.054826136,0.1745446156\H,2.1906824654,1.2513879802,0.4260969
133\H,1.4257394134,0.1102726037,2.2607259011\N,2.158564139,-2.16109731
04,-1.9295717807\C,0.8791699593,-2.5743233996,-2.4853661313\H,0.205565
7223,-2.9057078125,-1.6898323915\H,0.3722500001,-1.7742861784,-3.05238
73011\H,1.0383676157,-3.417882746,-3.1636431248\C,3.027560866,-1.64936
89536,-2.9742101968\H,3.1895219603,-2.4321301641,-3.7215027972\H,2.616
8337921,-0.7673537809,-3.4983627871\H,3.9987337481,-1.3797205992,-2.54
91520417\Version=ES64L-G09RevE.01\State=1-A\HF=-711.7331962\RMSD=8.36
1e-09\RMSE=2.010e-06\Dipole=1.4386404,0.0790005,1.0001107\Quadrupole=-
8.183785,2.0109061,6.1728789,6.6120656,-4.0275132,3.4124967\PG=C01 [X(
C13H19N1O2)]\@

5h(iv) [product]

1\1\GINC-R388\FOpt\RM062X\6-31+G(d,p)\C13H20N1O2(1+)\ROOT\08-Aug-2017\0
0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdi
sk=2147483648\|a1\1,1\C,-0.4234505399,0.0479097391,-1.1763808668\C,-0
.8176599089,1.2549329216,-0.2670019033\C,0.9454365639,-0.5582195744,-0
.8174640342\C,2.0588025489,0.4875646901,-0.7542401085\C,1.608555557,1.
8151375208,-0.1179426461\C,0.3134322378,1.6613300486,0.6824456275\C,-1
.5250168923,-1.0565896098,-1.0265172105\C,-2.1055930178,0.8573965273,0
.4899684934\C,-3.1860027867,0.567074114,-0.5202048748\C,-2.8744312734,
-0.4468534549,-1.3266830792\H,1.1880698639,-1.334554516,-1.5496328872\
H,0.8584951717,-1.0607153107,0.1521100955\H,2.457171802,0.6737413661,-
1.7570274783\H,1.4335756894,2.5304125298,-0.9286644772\H,0.0646759431,
2.6098884291,1.1670293856\H,0.4171891098,0.9154090973,1.4800209254\H,-
4.1000840314,1.1472855126,-0.5639211321\H,-3.506036937,-0.8339291505,-
2.1180347632\H,-1.2935896631,-1.9460565068,-1.612448634\H,-2.388271231
1,1.593438346,1.2426547288\O,-1.7943155332,-0.3470477494,1.2347477631\
C,-1.4839724527,-1.4046470539,0.4540237547\O,-1.1151765225,-2.44795800
42,0.9250074585\H,2.4123742202,2.2532472249,0.4868371349\H,-0.41114279
42,0.359765565,-2.2254650441\H,-1.0592040074,2.1168419397,-0.897819171
4\N,3.2732455392,-0.0770160933,-0.0024933522\C,3.0626687221,-0.3164027
805,1.462809431\H,2.7049106238,0.5972352759,1.9336229232\H,2.340227392
5,-1.1205811816,1.5963941921\H,4.0188769873,-0.6083733039,1.8974210174
\C,3.8273261923,-1.3038080961,-0.6575407214\H,4.790943044,-1.536977583
4,-0.2045881318\H,3.1344591337,-2.1288345161,-0.495192688\H,3.94784579
, -1.1141907012,-1.724402115\H,3.9907654589,0.651064339,-0.0761976117\
Version=ES64L-G09RevE.01\State=1-A\HF=-712.1129037\RMSD=1.513e-09\RMSE
=3.177e-06\Dipole=4.2861217,1.4411555,-1.0997875\Quadrupole=25.6822399
, -13.7930197,-11.8892202,-6.3819084,5.5917506,5.6478948\PG=C01 [X(C13H
20N1O2)]\@

7a(ii)[transition state]

1\1\GINC-R520\FTS\RM062X\6-31+G(d,p)\C11H13O2(1-)\ROOT\07-Aug-2017\0\0
#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcf
c,noeigentest,maxcyc=200) maxdisk=1610612736\|a2\|-1,1\C,1.2315795088,
-0.192068401,1.2722228664\C,1.4564002649,0.915286646,0.4593350852\C,1.
1729155534,-1.4501143068,0.4274473421\C,1.5647180485,0.4797572216,-0.9
892346479\C,-0.8211716795,0.2115647692,2.0356157018\C,-0.4489765287,2.
0448444536,0.689858014\C,-1.3385527022,1.1890401479,0.0450521823\C,-1.
5660492141,0.0684763372,0.867625663\C,-0.4616978058,1.6717896128,2.151
1964989\H,0.3931743964,-2.1556822729,0.739576611\H,2.1421530889,-1.965
5715209,0.4759337086\H,1.0658426339,1.1576503925,-1.6926761659\H,2.624
9950444,0.4127303471,-1.2699278534\H,-1.6577001987,1.277363549,-0.9872
99324\H,-2.0859899277,-0.8321977631,0.5612696558\H,0.4573878784,1.8878
503945,2.6997191294\H,-1.296380054,2.2010083641,2.6412825306\H,-0.8857
095298,-0.4555502405,2.8895872573\H,-0.1776305345,3.0322007166,0.32933
89335\C,0.971807991,-0.9455997657,-1.01789717\H,-0.0936375819,-0.90516
18575,-1.2574796187\H,1.5720455606,-0.2279797858,2.3050355341\H,1.9831
625557,1.7969877803,0.8185473792\C,1.6684526794,-1.8623831171,-2.07415

55158\O,0.9220833261,-2.3548687932,-2.9516769173\O,2.9070582265,-2.000
4189077,-1.9194698802\Version=ES64L-G09RevE.01\State=1-A\HF=-577.1910
802\RMSD=9.503e-09\RMSF=8.019e-07\Dipole=-1.911524,3.2704102,3.9265412
\Quadrupole=2.2466026,2.2456272,-4.4922298,11.4108714,10.9947641,-19.2
523748\PG=C01 [X(C11H13O2)]\@

7a(i) [transition state]

1\1\GINC-R543\FTS\RM062X\6-31+G(d,p)\C11H14O2\ROOT\07-Aug-2017\0\#M06
2X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,no
eigentest,maxcyc=200) maxdisk=1610612736\|a4\|0,1\C,1.4906700412,0.236
9224963,1.101504553\C,1.2610490838,1.2145274358,0.1381770267\C,1.66920
44726,-1.1205069131,0.4511608977\C,1.2611479766,0.6048289087,-1.249816
7699\C,-0.4390305745,0.1947205128,2.18612144\C,-0.8225071549,1.8257645
335,0.6033695388\C,-1.5178849414,0.6740006085,0.2384209826\C,-1.284578
0301,-0.3221446366,1.2050018734\C,-0.5006823673,1.695460245,2.06929213
13\H,1.1596867915,-1.9407471259,0.9654339787\H,2.738143207,-1.37218280
89,0.4077851417\H,0.4700663225,0.9866015173,-1.9034744322\H,2.21899344
89,0.7925937679,-1.7505714091\H,-2.0411600549,0.527836251,-0.700255121
3\H,-1.5993960641,-1.357262897,1.1292689414\H,0.3816672728,2.237112414
2,2.4134850079\H,-1.3719900245,2.0476926655,2.6437400688\H,-0.18662088
32,-0.3210073775,3.1069767398\H,-0.9138080822,2.7803702123,0.095618089
8\C,1.1084199566,-0.9000779983,-0.9804294681\H,0.0528498783,-1.1862069
953,-0.9832967132\H,1.9928658279,0.450418701,2.039730329\H,1.566399181
,2.2470082986,0.2737244207\C,1.8110941346,-1.7744342743,-1.9842250959\
O,2.5906189781,-1.4142814831,-2.8331314598\O,1.4932412799,-3.077128621
6,-1.8132453862\H,2.0007513237,-3.5840484366,-2.4655203055\Version=ES
64L-G09RevE.01\State=1-A\HF=-577.7512837\RMSD=3.676e-09\RMSF=2.477e-06
\Dipole=-0.2904341,0.002638,0.6571087\Quadrupole=-4.0252869,5.6300475,
-1.6047606,-0.8166787,4.8810725,2.158052\PG=C01 [X(C11H14O2)]\@

7a(iii) [transition state]

1\1\GINC-R277\FTS\RM062X\6-31+G(d,p)\C12H19N1\ROOT\07-Aug-2017\0\#M06
2X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,no
eigentest,maxcyc=200) maxdisk=1610612736\|a6\|0,1\C,1.5274104574,0.261
7941261,1.031490006\C,1.1864635553,1.0833288344,-0.0384963135\C,1.7304
132169,-1.1613039833,0.5558236888\C,1.1326777863,0.2791549678,-1.32032
85345\C,-0.3213695503,0.3151307812,2.2553868235\C,-0.8858769989,1.6760
595189,0.4829746362\C,-1.5506775202,0.4587731829,0.3435739575\C,-1.205
9368426,-0.3722422854,1.4257802396\C,-0.4599207828,1.7788380268,1.9248
132444\H,1.3068875053,-1.9133297724,1.2309509203\H,2.8054946177,-1.368
4864586,0.4520770153\H,0.2880287686,0.5419318464,-1.9670366846\H,2.057
8529714,0.4332331749,-1.8946105959\H,-2.1244239498,0.1523715461,-0.524
1250166\H,-1.4724719923,-1.418976701,1.5220928819\H,0.4190439131,2.395
6816163,2.1185135753\H,-1.3045113108,2.1835863647,2.50455323\H,0.01800
536,-0.047791454,3.2201721102\H,-1.0560104219,2.5405848059,-0.15054556
22\C,1.0845079085,-1.1882554934,-0.8453479977\H,0.0247389966,-1.492636
9762,-0.7414058944\H,2.0757106106,0.6259184773,1.8946479956\H,1.449214
7339,2.1359877486,-0.07220458\N,1.7593013679,-2.1038399835,-1.76337053
26\C,1.7292372871,-3.4663054262,-1.2544155769\H,2.2302354053,-4.131110
5695,-1.9632449493\H,2.2569716156,-3.5295345811,-0.3004291047\H,0.6947
478269,-3.8335145793,-1.1057146776\C,1.146829066,-2.0627846907,-3.0822
50694\H,0.0742162831,-2.3380557307,-3.0530152393\H,1.2335768681,-1.062
9580471,-3.5128479776\H,1.662293248,-2.7628902857,-3.7452383931\Versi
on=ES64L-G09RevE.01\State=1-A\HF=-523.1414057\RMSD=4.346e-09\RMSF=4.38
0e-06\Dipole=-0.0884705,0.0782018,0.0882515\Quadrupole=-4.6969277,3.03
04597,1.666468,0.6441522,2.6843152,0.4513879\PG=C01 [X(C12H19N1)]\@

7a(iv) [transition state]

1\1\GINC-R304\FTS\RM062X\6-31+G(d,p)\C12H20N1(+)\ROOT\07-Aug-2017\0\#
M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc
noeigentest,maxcyc=200) maxdisk=1610612736\|a3\|1,1\C,1.4032727661,0
.0295535984,1.112681425\C,1.3568697085,1.0289261382,0.1453925551\C,1.4
434399611,-1.3378702159,0.4608704082\C,1.361665869,0.4231939844,-1.243
6268853\C,-0.5759184402,0.2433995378,2.0865648511\C,-0.6528971227,1.89
96312742,0.4833640071\C,-1.4682397789,0.8419509312,0.0767974481\C,-1.4
21284211,-0.1683987735,1.0548000413\C,-0.43215856,1.7361839647,1.96286
88877\H,0.8194358261,-2.0869308815,0.9581225449\H,2.4796227667,-1.7160

746225,0.4541971334\H,0.6801165375,0.9133338992,-1.9457579631\H,2.3777
359405,0.4780716445,-1.6694774206\H,-1.9824528445,0.77652103,-0.876469
8234\H,-1.8932455144,-1.1427002802,0.9812953157\H,0.4840073513,2.16898
38078,2.3660010139\H,-1.2871423191,2.1975779007,2.4805869651\H,-0.4528
651135,-0.2913465963,3.0226294645\H,-0.5991738374,2.8568214944,-0.0247
832359\C,0.9759982473,-1.0401307894,-0.9730509243\H,-0.1041261945,-1.1
827867367,-1.0686206281\H,1.8759442704,0.1634314776,2.0784414369\H,1.7
900773565,2.011548325,0.2896786667\N,1.586652577,-1.9894235832,-1.9831
387658\C,1.2666829895,-3.4172859551,-1.6737579716\H,1.7292195694,-4.05
53217768,-2.4265797165\H,1.6471627737,-3.6653796294,-0.6846652663\H,0.
1820874884,-3.5325026601,-1.6992927957\C,1.1847144245,-1.6508839333,-3
.3833949682\H,0.0982112152,-1.7248470674,-3.449084057\H,1.5064864801,-
0.6373221426,-3.6152875801\H,1.6507103801,-2.3601152719,-4.0672144853\
H,2.6044794371,-1.8748140923,-1.9135206777\Version=ES64L-G09RevE.01\St
ate=1-A\HF=-523.5272601\RMSD=8.884e-09\RMSF=2.119e-06\Dipole=1.375572
3,-2.1306912,-2.2673967\Quadrupole=-8.8650597,3.836112,5.0289476,-4.99
56503,-5.0517459,11.0003682\PG=C01 [X(C12H20N1)]\@

8a(ii) [transition state]

1\1\GINC-R412\FTS\RM062X\6-31+G(d,p)\C12H15O2(1-)\ROOT\07-Aug-2017\0\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc, noeigentest,maxcyc=200) maxdisk=1610612736\|a1\|-1,1\C,1.1789129378,
-0.1626480208,1.0614165918\C,1.0944958084,0.7671011048,0.0218191038\C,
0.8732703681,-1.6364158756,0.8468711112\C,0.9147641786,-2.0315232702,-
0.6314166059\C,0.0925709071,-1.0375579771,-1.4539836722\C,0.7399370968
,0.3467877252,-1.3914155964\C,-0.4452960695,0.6040622414,2.4352349576\
C,-0.543578211,2.0535758211,0.6516262418\C,-1.6342426976,1.1840345484,
0.5816282807\C,-1.5695115201,0.2967109047,1.6724556019\C,-0.0433740292
,2.0103183552,2.074062204\H,-0.1135044813,-1.888294872,1.2598222752\H,
1.627297403,-2.2226502318,1.3791472057\H,0.468398496,-3.0310602348,-0.
7381110705\H,-0.9360278102,-0.9914400029,-1.0646882955\H,0.1033849751,
1.1009732489,-1.8746426238\H,1.6723487698,0.2923308792,-1.9689254784\H
,-2.3105598268,1.0942816935,-0.2611980004\H,-2.1909936851,-0.583119444
6,1.796584245\H,1.0135535072,2.247407898,2.2076414947\H,-0.6423888319,
2.7145007988,2.6765900747\H,-0.1968613074,0.1362298085,3.3825549478\H,
-0.4063589232,2.912108836,0.0006216923\H,0.0572777495,-1.3683678229,-2
.4952884735\H,1.8872135554,0.0596088996,1.8562103907\H,1.756814539,1.6
299817099,0.0861821958\C,2.3787923866,-2.1648836791,-1.1901782041\O,3.
2896229828,-2.2968737907,-0.3400446478\O,2.4678217321,-2.1522492509,-2
.4421359461\Version=ES64L-G09RevE.01\State=1-A\HF=-616.4903523\RMSD=8
.846e-09\RMSF=5.653e-06\Dipole=-3.2528255,2.8339752,2.3093508\Quadrupo
le=-6.6636523,4.299393,2.3642593,18.7462375,13.3059518,-11.3334949\PG=
C01 [X(C12H15O2)]\@

8a(i) [transition state]

1\1\GINC-R425\FTS\RM062X\6-31+G(d,p)\C12H16O2\ROOT\07-Aug-2017\0\#M06
2X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,no
eigentest,maxcyc=200) maxdisk=1610612736\|a1\|0,1\C,1.3497605867,0.151
0547221,1.0621292406\C,1.097720547,1.1109783859,0.0758643585\C,1.42578
5095,-1.328973946,0.7404354228\C,0.7760904919,-1.6647511,-0.5989878544
\C,1.2966348427,-0.709392915,-1.6860741686\C,0.8349733964,0.7156570907
,-1.3693173452\C,-0.358169395,0.3383591969,2.3635311975\C,-0.834927323
2,1.9720212759,0.8164389446\C,-1.680199184,0.88531171,0.5917128919\C,-
1.392305619,-0.1133721144,1.5368404588\C,-0.3180391561,1.8384908784,2.
223552566\H,0.9814296128,-1.9350803545,1.5376811016\H,2.4805079286,-1.
6290872682,0.6869034572\H,-0.3141654888,-1.5451513496,-0.5416134287\H,
0.9318759981,-1.0162006181,-2.6708727948\H,-0.2333966164,0.7843375799,
-1.6067420081\H,1.344847673,1.4223796401,-2.0329434834\H,-2.3521547716
,0.7733251639,-0.2518487472\H,-1.8084600307,-1.1148621521,1.5431722225
\H,0.6455564744,2.3090898423,2.4245281019\H,-1.0660982855,2.2667273978
,2.909084413\H,-0.0267975223,-0.182643218,3.2567347031\H,-0.9069515481
,2.9211084527,0.2950994074\H,2.3929310307,-0.7617674596,-1.7019184062\
H,1.9856491204,0.4537180683,1.8909891106\H,1.5367601006,2.0941430585,0
.2194064647\C,1.0438138595,-3.098788265,-0.9852875534\O,1.8491884352,-
3.8381734962,-0.4721216005\O,0.2747882377,-3.4922293049,-2.0247124272\
H,0.5200315099,-4.406908902,-2.2321442449\Version=ES64L-G09RevE.01\St
ate=1-A\HF=-617.0490524\RMSD=4.219e-09\RMSF=5.742e-06\Dipole=-0.252625

4,0.5839441,-0.1954637\Quadrupole=-3.8718423,0.6445146,3.2273277,5.043
2105,0.8909981,2.8954398\PG=C01 [X(C12H16O2)]\@

8a(iii) [transition state]

1\1\GINC-R450\FTS\RM062X\6-31+G(d,p)\C13H21N1\ROOT\07-Aug-2017\0\#M06
2X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcf, no
eigentest,maxcyc=200) maxdisk=1610612736\|a6\|0,1\C,1.4671417102,0.238
5950277,0.9937562081\C,1.0475082732,1.1182668172,-0.0077633801\C,1.638
9155368,-1.2487244688,0.7438606904\C,0.9645295339,-1.7493475286,-0.539
8164748\C,1.3145175409,-0.7787407933,-1.669879966\C,0.7126662133,0.602
0353049,-1.3952400754\C,-0.136856191,0.368938169,2.437314775\C,-0.8787
630058,1.8506557466,0.8434804361\C,-1.6399012188,0.6842579562,0.757018
6764\C,-1.1881315321,-0.2224020364,1.7296593546\C,-0.2421466477,1.8546
511896,2.2079146147\H,1.2784570491,-1.807211959,1.6130094824\H,2.71291
97958,-1.4699867776,0.6480061484\H,-0.1377506595,-1.7280615301,-0.3935
124704\H,0.9393606923,-1.1342254088,-2.6324801879\H,-0.3728973144,0.53
55080819,-1.5373711477\H,1.0773309777,1.3149487781,-2.1427429424\H,-2.
3616438715,0.4589312984,-0.0199905828\H,-1.5045703749,-1.255591638,1.8
222572003\H,0.6894656088,2.4156620366,2.2973192452\H,-0.9677621182,2.2
640620778,2.9281585607\H,0.3135613754,-0.0631158178,3.3259860747\H,-1.
0795507969,2.7547806233,0.2776663889\H,2.4080749559,-0.7194637035,-1.7
452154669\H,2.1415460764,0.6340167377,1.7502106861\H,1.4095139231,2.14
1296001,0.0444215622\N,1.3861043512,-3.1236862675,-0.8475726343\C,1.18
04747518,-4.0262671153,0.2775775818\H,1.4189131954,-5.0456294392,-0.03
53814486\H,1.8404517272,-3.7756283129,1.1089552307\H,0.1340912272,-4.0
14450977,0.6418339565\C,0.6897246148,-3.6568998481,-2.0107809945\H,-0.
410734741,-3.6286617194,-1.8899725515\H,0.9525713736,-3.1088016132,-2.
9156190485\H,0.9889929681,-4.6970538918,-2.1609785015\Version=ES64L-G
09RevE.01\State=1-A\HF=-562.4357464\RMSD=3.467e-09\RMSF=1.893e-06\Dipo
le=-0.071386,0.1082141,0.0894594\Quadrupole=-4.0463521,2.8057247,1.240
6273,2.1396432,3.20073,-0.3250427\PG=C01 [X(C13H21N1)]\@

8a(iv) [transition state]

1\1\GINC-R482\FTS\RM062X\6-31+G(d,p)\C13H22N1(1+)\ROOT\07-Aug-2017\0\|
#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcf
c,noeigentest,maxcyc=200) maxdisk=1610612736\|a4\|1,1\C,1.4180096452,0
.1671887599,0.943916413\C,1.0649875328,1.1088415527,-0.0287523193\C,1.
5264965016,-1.3120784984,0.6119319318\C,0.7777338171,-1.6264048536,-0.
6762356483\C,1.2241698831,-0.7076958658,-1.8025364267\C,0.7387316332,0
.7092053158,-1.4602872277\C,-0.2150394698,0.2915861873,2.3591221853\C,
-0.8417503647,1.8845910825,0.8219835304\C,-1.6563950886,0.7623284216,0
.6580889786\C,-1.2798831218,-0.2091652962,1.5996196959\C,-0.2376276984
,1.7878857958,2.1956152067\H,1.1366195799,-1.9261145761,1.4354947196\H
,2.589665369,-1.5647393209,0.4914397662\H,-0.2978868355,-1.5012032199,
-0.5057045916\H,0.8133478731,-1.0121548775,-2.7717334848\H,-0.33853134
69,0.7584987075,-1.6534356008\H,1.2089346526,1.4153394978,-2.150014383
\H,-2.3922735124,0.6284066601,-0.1272911165\H,-1.6879497226,-1.2123731
911,1.673504683\H,0.7120509029,2.3031953833,2.3424858442\H,-0.96559000
97,2.1927542091,2.9151493268\H,0.1813344694,-0.2004346775,3.2424558859
\H,-0.9870780278,2.8242055691,0.2993063175\H,2.3179353352,-0.717256903
, -1.8770799612\H,2.1021672946,0.4814784736,1.7260519041\H,1.4743658255
,2.1070434766,0.0858821845\N,0.9365221157,-3.1104630817,-1.0192341107\
C,-0.1832720063,-3.6142405318,-1.8723766888\H,-0.0358670078,-4.6777273
9,-2.0609513265\H,-1.1259612604,-3.4494613823,-1.3515654167\H,-0.17458
46189,-3.0659298113,-2.8141059952\C,2.259575209,-3.4616692121,-1.62364
35529\H,2.303690175,-3.0407351905,-2.6274223493\H,3.0606089663,-3.0546
385,-1.0089298232\H,2.340014365,-4.5475819406,-1.6716148049\H,0.877198
9453,-3.6035627726,-0.1221057456\Version=ES64L-G09RevE.01\State=1-A\H
F=-562.8231707\RMSD=6.381e-09\RMSF=7.129e-06\Dipole=0.8228025,-3.13962
54,-1.5016587\Quadrupole=-9.7247974,13.5191859,-3.7943886,-3.7592121,-
0.6121073,10.5481081\PG=C01 [X(C13H22N1)]\@

7b(ii) [transition state]

1\1\GINC-R871\FTS\RM062X\6-31+G(d,p)\C11H13O2(1-)\ROOT\07-Aug-2017\0\|
#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcf
c,noeigentest,maxcyc=200) maxdisk=1610612736\|a2\|-1,1\C,1.0136391467,
0.1541621118,1.2099668275\C,0.8455526459,1.1011221343,0.2001781358\C,0

.8832199356,-1.2512864643,0.6510929138\C,0.5865884383,0.4208482617,-1.1321198125\H,-0.0708852041,-1.6819724888,0.9910157852\H,1.6820085978,-1.9371838103,0.9511377066\H,-0.4695590522,0.5655887838,-1.4059063162\H,1.1977392968,0.793249679,-1.9605868256\C,3.1305707795,0.4525426566,1.7633503802\C,2.8532077583,2.0153554721,0.0973125021\C,3.5923582152,0.9470208676,-0.4111998574\C,3.7621055772,-0.0093092108,0.6082875127\C,2.9435182071,1.9410190715,1.6016612895\H,3.190975621,-0.0367167598,2.7313502707\H,2.662772598,2.9393276752,-0.441255043\H,3.8113587823,0.7640137828,-1.4569822436\H,4.1274136343,-1.0160843036,0.4407308137\H,3.8671980475,2.4493497577,1.9247368448\H,2.1001405766,2.3724102959,2.1467308279\C,0.902192209,-1.0723661516,-0.884552666\H,0.1258913027,-1.6984366599,-1.3424825519\H,0.7468446242,0.3589742085,2.2443203772\H,0.4394394615,2.0905901711,0.3977456397\C,2.2191365571,-1.5786593598,-1.5782370795\O,2.5259979135,-1.0053586715,-2.6504638632\O,2.7972053305,-2.5389970493,-1.0160345686\Version=ES64L-G09RevE.01\State=1-A\HF=-577.1944489\IRMSD=9.036e-09\IRMSF=7.578e-06\Dipole=-1.1243777,2.5245408,2.5538674\Quadrupole=5.4197653,-2.6904978,-2.7292674,3.2785274,3.0720142,-8.1181045\PG=C01 [X(C11H13O2)]\@

7b(i) [transition state]

1\1\GINC-R882\FTS\RM062X\6-31+G(d,p)\C11H14O2\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,no eigentest,maxcyc=200) maxdisk=1610612736\|a3\0,1\C,0.9813483344,0.1707771905,1.1765494548\C,0.8664661289,1.1208193153,0.1668093654\C,0.8110549873,-1.2321070953,0.6236946197\C,0.5880075632,0.463685694,-1.1702694084\H,-0.1497649563,-1.6442470876,0.9530382505\H,1.5909375344,-1.9330841934,0.9354297813\H,-0.455663421,0.6385653748,-1.4565023759\H,1.2113171761,0.8364480326,-1.9874146309\C,3.1016479923,0.4118627555,1.785889723\C,2.9100205237,1.9431544652,0.0759421801\C,3.623230002,0.8367605756,-0.3880156842\C,3.7397194392,-0.0991564116,0.6564596706\C,2.964469478,1.8974016501,1.5806343045\H,3.1313273675,-0.0538942423,2.7655521703\H,2.7755965308,2.8612793746,-0.48714516\H,3.9207570268,0.6705892175,-1.4176647716\H,4.129038547,-1.1049300681,0.5543223684\H,3.9029228717,2.3751427798,1.903733999\H,2.1352376879,2.3772558141,2.1031121476\C,0.8102856473,-1.0505699159,-0.9117137872\H,-0.007641919,-1.6234335025,-1.3670020415\H,0.7016195091,0.3767084768,2.2044347726\H,0.4943511656,2.1232559368,0.3522052601\C,2.0369550397,-1.6396732015,-1.5759182221\O,2.7516698531,-2.4981725923,-1.115990159\O,2.2218156839,-1.166954015,-2.8281993181\H,2.9749392065,-1.6497933277,-3.2019075093\Version=ES64L-G09RevE.01\State=1-A\HF=-577.7499666\IRMSD=7.998e-09\IRMSF=8.712e-06\Dipole=-0.4600732,0.5306072,-0.1011278\Quadrupole=-1.1448896,-2.642495,3.7873846,0.8059479,-1.9486748,1.7928423\PG=C01 [X(C11H14O2)]\@

7b(iii) [transition state]

1\1\GINC-R924\FTS\RM062X\6-31+G(d,p)\C12H19N1\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,no eigentest,maxcyc=200) maxdisk=1610612736\|a6\0,1\C,1.211446308,0.0213144757,1.3117643257\C,0.8243570629,0.9249229778,0.3226250051\C,1.4535068236,-1.3430328847,0.6917529595\C,0.7824710373,0.2234092792,-1.0229396039\H,1.1042929267,-2.1575716265,1.3337416497\H,2.5181975307,-1.510316754,0.4785716524\H,-0.058721217,0.557356896,-1.6381193438\H,1.7068665576,0.3836386139,-1.5946257026\C,3.1615558215,0.8666456319,1.9641910323\C,2.5211040521,2.3616083608,0.3277338054\C,3.5356310944,1.5500205634,-0.1762326515\C,3.926230443,0.6382787207,0.8218157678\C,2.5730947874,2.2476006715,1.8296366368\H,3.3348909931,0.3854825229,2.9211147771\H,2.1178662866,3.2264318365,-0.1887392482\H,3.8806236047,1.536469213,-1.2036567208\H,4.6177671107,-0.184175422,0.6798614085\H,3.3098667275,2.9748661037,2.2056590659\H,1.6291035566,2.4144457243,2.3515035845\C,0.7006907292,-1.2708035473,-0.6518039124\H,-0.3653595912,-1.5251942947,-0.4670134642\H,0.8839423107,0.1079500905,2.3420241748\H,0.1728127934,1.7680113428,0.524850393\N,1.2505002201,-2.1536971604,-1.6734606543\C,1.205175632,-3.5431083776,-1.246695391\H,1.6157765682,-4.1798052409,-2.0350825345\H,1.8097654556,-3.6855706653,-0.3483847744\H,0.1729198145,-3.8815711835,-1.0304109683\C,0.5442043406,-2.0006297799,-2.9353454638\H,-0.5358368438,-2.227674055,-2.8412599161\H,0.6503666446,-0.980241801,-3.3099372743\H,0.9730744188,-2.6795562316,-3.6774096143\Version=ES64L-G09RevE.01\State=1-A\HF=-523.1375996\IRMSD=3.264e-09\IRMSF=3.108e-06\Dip

ole=-0.3101577,0.0151844,0.1352641\Quadrupole=-3.2149705,1.3341016,1.8
808689,-1.7302134,0.412865,0.1795861\PG=C01 [X(C12H19N1)]\@

7b(iv) [transition state]

1\1\GINC-R931\FTS\RM062X\6-31+G(d,p)\C12H20N1(1+)\ROOT\07-Aug-2017\0\
#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcf
c,noeigentest,maxcyc=200) maxdisk=1610612736\|a6\|1,1\C,1.1970954129,0
.022801252,1.3049476508\C,0.7953807396,0.9345811587,0.3288602404\C,1.4
18503437,-1.3438073673,0.6814569889\C,0.7168699213,0.2489593656,-1.023
5998443\H,1.0684080718,-2.1607365463,1.3176516407\H,2.4854468245,-1.51
49768041,0.4646454473\H,-0.1391570046,0.5805409976,-1.6168631954\H,1.6
297862818,0.4273961123,-1.6147041359\C,3.1707289176,0.8474664934,1.916
7001202\C,2.5057270996,2.3573279755,0.3004931606\C,3.4983452235,1.5352
268522,-0.2316896448\C,3.9037481431,0.6148634341,0.7535053257\C,2.5857
299332,2.2291140251,1.7979858519\H,3.368421113,0.3648685391,2.86792258
99\H,2.1053916351,3.2319734392,-0.2010405788\H,3.8501227092,1.55593676
59,-1.2574769681\H,4.6184464265,-0.1881980359,0.6095799508\H,3.3414473
627,2.9449645456,2.1558211284\H,1.6614919575,2.4108948227,2.348068905\
C,0.6352288811,-1.2343270914,-0.6347828076\H,-0.4051425557,-1.55029124
46,-0.5018005085\H,0.8876060054,0.0938501378,2.3401155344\H,0.14677215
05,1.7755343448,0.5398264083\N,1.1928789782,-2.1441428059,-1.714228454
5\C,1.1899096671,-3.5788685767,-1.2950309661\H,1.5997809927,-4.1855596
779,-2.1023951684\H,1.7930784895,-3.692179383,-0.3960798672\H,0.157798
0658,-3.8704733726,-1.0946148125\C,0.4811282365,-1.9702148661,-3.01704
53079\H,-0.5702049994,-2.2185475762,-2.8637974939\H,0.5786103378,-0.93
69128382,-3.3450043146\H,0.9204302206,-2.6422150647,-3.7541595214\H,2.
1698453245,-1.8576390108,-1.8487163535\Version=ES64L-G09RevE.01\State
=1-A\HF=-523.5243386\RMSD=5.839e-09\RMSF=6.153e-06\Dipole=-0.949793,-2.
.521802,-1.964937\Quadrupole=-9.6071026,7.1293767,2.4777259,3.1093093,
4.1787123,11.4639011\PG=C01 [X(C12H20N1)]\@

8b(ii) [transition state]

1\1\GINC-R934\FTS\RM062X\6-31+G(d,p)\C12H15O2(1-)\ROOT\07-Aug-2017\0\
#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcf
c,noeigentest,maxcyc=200) maxdisk=1610612736\|a4\|1,1\C,1.1018352616,
0.0836595453,1.1760998221\C,0.8393358861,1.0280105655,0.1855068942\C,1
.4264756876,-1.3058739577,0.6935994761\C,0.3491155976,-1.820916126,-0.
2967374684\C,-0.0020401899,-0.7502334858,-1.3512424115\C,0.8808832857,
0.5109824507,-1.2316323983\H,1.5332408658,-2.0193033834,1.5147530865\H
.2.3832774433,-1.2894037333,0.15381798\H,-0.5396280288,-2.0791277016,0
.2909149119\H,-1.0529135069,-0.4479308466,-1.248699215\H,0.5697058745,
1.2844317374,-1.9442023444\H,1.9080382724,0.2271941267,-1.4935681086\C
.3.0048091465,0.8963221733,2.0705785246\C,2.5635522509,2.4315944898,0.
4034220484\C,3.6143018734,1.6135954963,-0.0046476313\C,3.8802128412,0.
6739983553,1.0125518734\C,2.4547034772,2.2901186694,1.9015063556\H,3.0
51881977,0.3835823658,3.0255938159\H,2.2237962275,3.3095404728,-0.1371
608733\H,4.0471710642,1.5949084326,-0.9983529259\H,4.5450541423,-0.176
666356,0.916996591\H,3.1555896933,3.0015600397,2.3703237492\H,1.45999
41091,2.4576334519,2.3194340781\H,0.1364516611,-1.1968118063,-2.340298
4935\H,0.6433308517,0.1975623236,2.1569649053\H,0.1724750676,1.8605138
374,0.4043372368\C,0.904981029,-3.1583885158,-0.8985794624\O,0.8547589
692,-4.1362291509,-0.1157969834\O,1.3833281698,-3.0960034701,-2.056241
1014\Version=ES64L-G09RevE.01\State=1-A\HF=-616.4877486\RMSD=3.976e-0
9\RMSF=1.302e-05\Dipole=0.4602449,5.2190433,1.9430007\Quadrupole=14.49
51347,-24.1116261,9.6164915,-8.6711322,-2.1404768,-12.4368071\PG=C01 [
X(C12H15O2)]\@

8b(i) [transition state]

1\1\GINC-R935\FTS\RM062X\6-31+G(d,p)\C12H16O2\ROOT\07-Aug-2017\0\#M06
2X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcf,c,no
eigentest,maxcyc=200) maxdisk=1610612736\|a1\|0,1\C,0.9434810176,0.121
3096758,1.0343709247\C,0.9154853981,1.0912658889,0.0358737835\C,1.2345
288843,-1.2842971346,0.5772287523\C,0.2713532268,-1.6830916412,-0.5833
114619\C,0.1732750748,-0.5797582246,-1.6607646721\C,1.1313851704,0.592
3283368,-1.3732143477\H,1.1540927196,-2.0064474142,1.393792227\H,2.261
3828685,-1.3375637546,0.1921020976\H,-0.7101973138,-1.8828908026,-0.14
19662081\H,-0.8522965842,-0.1989410888,-1.6895140966\H,0.9838210605,1.

3918848245,-2.1052414472\H,2.1622539155,0.2370326941,-1.4929021492\C,2.7507318195,0.7460282433,2.2207242253\C,2.6844623245,2.3291912893,0.5409258286\C,3.712251595,1.4274005048,0.2710028166\C,3.751846404,0.4620366541,1.2956673424\C,2.3448139265,2.1800891302,2.0019252014\H,2.6236396552,0.227830641,3.1654242509\H,2.5099156973,3.2413309894,-0.0202597891\H,4.3022859537,1.4000085709,-0.6379984967\H,4.3769892243,-0.4237249453,1.2969283572\H,3.0299852869,2.8208717892,2.5791246646\H,1.3207100821,2.4331947562,2.2810605863\H,0.3951267379,-1.0072661778,-2.6423433805\H,0.3484360224,0.2482374964,1.9342764899\H,0.2925248054,1.9722717251,0.1668359336\C,0.7747446033,-2.9899363777,-1.1500769153\O,1.3900990804,-3.1377457705,-2.1789943308\O,0.5074710567,-4.0269785365,-0.3254960907\H,0.8989302865,-4.8187513416,-0.725180096\Version=ES64L-G09RevE.01\State=1-A\HF=-617.0469295\RMSE=3.593e-09\RMSE=2.270e-06\Dipole=-0.3335823,0.2827844,0.6353544\Quadrupole=-1.0614453,4.3503019,-3.2888566,-1.5346078,-0.0626264,-2.9861873\PG=C01 [X(C12H16O2)]\@

8b(iii) [transition state]

1\1\GINC-R105\FTS\RM062X\6-31+G(d,p)\C13H21N1\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,no eigentest,maxcyc=200) maxdisk=1610612736\|a6\|0,1\C,1.118796091,0.0604342631,1.1291820307\C,0.9433786081,0.9390939822,0.0651872301\C,1.4820603112,-1.3623302768,0.7742419116\C,0.473780024,-1.9148131272,-0.2544270717\C,0.3617990525,-0.9559482792,-1.4726455887\C,1.1749909052,0.3422032248,-1.299451133\H,1.4953883141,-1.9761642908,1.6782206863\H,2.4848540031,-1.4101105022,0.3280527669\H,-0.5095586891,-1.9605866813,0.259019393\H,-0.6884398846,-0.7049716551,-1.6568892392\H,0.9331718985,1.0518045161,-2.0967739171\H,2.2385972001,0.0954150094,-1.4069662142\C,2.910295236,0.9086620103,2.1395902226\C,2.61174418,2.3963151482,0.399489397\C,3.7027750606,1.580159093,0.1114653096\C,3.8850185521,0.6718702561,1.1720932181\C,2.3644095502,2.2897692834,1.8820126333\H,2.8883883541,0.4326236564,3.1145169357\H,2.3171187144,3.2559627496,-0.1932813654\H,4.2432466678,1.5614519589,-0.8281173005\H,4.587111983,-0.1541579711,1.1755563179\H,3.0168449965,3.0164286533,2.3916364934\H,1.3371178922,2.4632334091,2.2066947999\H,0.7342589727,-1.4798354246,-2.3587037604\H,0.5610016963,0.2131661947,2.0492625493\H,0.2492559659,1.7699515395,0.156212989\N,0.8268282457,-3.2660465675,-0.7152436315\C,1.1482957408,-4.176106642,0.3739192589\H,1.2972120429,-5.1784063076,-0.0362042811\H,2.0738217694,-3.8807583576,0.870346804\H,0.3414604537,-4.2326433224,1.1308406742\C,-0.2651987717,-3.8334632373,-1.4948320488\H,-1.1810035825,-3.9659652726,-0.8864983527\H,-0.5128350665,-3.1908151714,-2.3417157102\H,0.0318855119,-4.8099358615,-1.8867335532\Version=ES64L-G09RevE.01\State=1-A\HF=-562.4342275\RMSE=4.836e-09\RMSE=1.352e-06\Dipole=-0.3047206,0.0630713,0.185888\Quadrupole=-2.2531956,1.3951124,0.8580832,-1.4010352,0.0756396,-1.0614724\PG=C01 [X(C13H21N1)]\@

8b(iv) [transition state]

1\1\GINC-R868\FTS\RM062X\6-31+G(d,p)\C13H22N1(1+)\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,c,noeigentest,maxcyc=200) maxdisk=1610612736\|a6\|1,1\C,1.105672979,0.0652308584,1.1239926592\C,0.9289639461,0.9523307601,0.0661207856\C,1.4724678863,-1.3547176806,0.7530501939\C,0.4365450518,-1.8589423047,-0.2623268459\C,0.3216088883,-0.9191611776,-1.4902262939\C,1.1444833582,0.3724311064,-1.3108769571\H,1.4946168836,-1.9804176791,1.6481488919\H,2.4725330709,-1.3833487436,0.2938254638\H,-0.530393684,-1.9724492693,0.2397724045\H,-0.7294184607,-0.6702788983,-1.6599517036\H,0.8810474652,1.0836585034,-2.0972318981\H,2.2058197526,0.1316193093,-1.4463882251\C,2.9198888313,0.9002799659,2.1315450612\C,2.5937849493,2.3846230212,0.3922217612\C,3.6790889938,1.5635655615,0.0879732067\C,3.8772897439,0.6583674576,1.1469189985\C,2.3662851899,2.2764754994,1.8764126558\H,2.9162055622,0.429831217,3.1094153733\H,2.3021724751,3.2499630439,-0.1934073818\H,4.2236139513,1.5628636853,-0.8495880051\H,4.6022702249,-0.1481366685,1.156673932\H,3.0309380147,3.0010709058,2.3710942978\H,1.3481463154,2.4590367794,2.2227134262\H,0.6706548687,-1.4305582158,-2.3981206601\H,0.5568073247,0.19688324,2.05058702\H,0.2361596601,1.7814565648,0.1663422109\N,0.7585348927,-3.2760876687,-0.7523208667\C,1.1431576131,-4.2204514712,0.3415175552\H,1.2355475006,-5.2214034716,-0.0797585515\H,2.0906048364,-3.9112212167,0.7768058795\H,0.3565448819,-4.205435558,

1.0976300138\C,-0.3799047153,-3.848618061,-1.5384409943\H,-1.211373129
7,-4.008924177,-0.850697632\H,-0.6727516871,-3.1513590753,-2.320692308
9\H,-0.06938166,-4.7972353473,-1.9760857508\H,1.5631842251,-3.18780879
55,-1.3824427162\Version=ES64L-G09RevE.01\State=1-A\HF=-562.821508\RM
SD=3.835e-09\RMSF=-2.138e-06\Dipole=-1.2726263,-3.577348,-1.1197252\Qua
drupole=-10.1006801,16.8815017,-6.7808216,6.9998224,3.1709835,7.466214
6\PG=C01 [X(C13H22N1)]\@\

7c(ii) [transition state]

1\1\GINC-R146\FTS\RM062X\6-31+G(d,p)\C11H13O2(1-)\ROOT\07-Aug-2017\0\#\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc
c,noeigentest,maxcyc=200) maxdisk=1610612736\|a6\|-1,1\C,1.3408381319,
1.0520689229,0.335125044\C,0.864018569,0.1477858635,1.2840775142\C,1.6
212299702,0.3544718231,-0.9837921385\C,0.7746160518,-1.2511328198,0.70
11240589\H,2.6332472525,0.5459988665,-1.3646618404\H,0.9360524738,0.70
14070781,-1.7659611259\H,1.2880739486,-2.0051351147,1.3124866019\H,-0.
2680085515,-1.5821100649,0.6303522687\C,3.3640083543,1.5241120289,1.13
51750502\C,2.5772452871,0.0320116451,2.7009567077\C,2.541332569,1.3152
955493,3.2486544984\C,3.0224390337,2.2277098973,2.2911816808\C,3.52844
4107,0.0825833356,1.5356035836\H,3.8461162423,1.9573620483,0.264580137
\H,2.3496812087,-0.8805864734,3.2426652641\H,2.059793289,1.5845508585,
4.1828684218\H,2.9686388594,3.3081519882,2.3741544875\H,4.553251545,-0
.0505096058,1.9237121329\H,3.3580437278,-0.6525091974,0.7494831504\C,1
.357548176,-1.1494118822,-0.7292091427\H,2.2987035768,-1.7110387887,-0
.7914919115\H,1.0627752253,2.1005939104,0.3506384151\H,0.1934170641,0.
4518476279,2.0808234551\C,0.448190839,-1.8160678941,-1.8213695592\O,-0
.2338060329,-2.7912162892,-1.4295260337\O,0.539848082,-1.3234513135,-2
.9696287201\Version=ES64L-G09RevE.01\State=1-A\HF=-577.1896414\RMSD=4
.154e-09\RMSF=8.978e-07\Dipole=2.2721125,2.8372259,3.8452639\Quadrupol
e=7.9659185,3.0307748,-10.9966934,-14.172139,-16.3556441,-17.2276446\PG
G=C01 [X(C11H13O2)]\@\

7c(i) [transition state]

1\1\GINC-R264\FTS\RM062X\6-31+G(d,p)\C11H14O2\ROOT\07-Aug-2017\0\#\#M06
2X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,no
eigentest,maxcyc=200) maxdisk=1610612736\|a6\|0,1\C,1.5508746928,1.165
959541,0.1766610555\C,0.8382464325,0.4264797628,1.1159261455\C,1.78864
81048,0.3575407292,-1.0861867613\C,0.5177262943,-0.960156357,0.5890124
79\H,2.8303520524,0.3675431794,-1.4268812176\H,1.1798772645,0.75505934
97,-1.9060607257\H,0.7733061196,-1.7748161861,1.2749178668\H,-0.560572
5232,-1.0382408499,0.3996259552\C,3.5487389455,1.3259643415,1.14747457
44\C,2.3703992928,0.097064603,2.7005558723\C,2.4938145028,1.4076751458
,3.1641212208\C,3.2120558347,2.1566151993,2.2172909873\C,3.4284620324,
-0.0875182672,1.6473936497\H,4.1918431331,1.6150169773,0.3223322146\H,
1.9500764614,-0.722285808,3.2750854715\H,1.9908719118,1.8146276572,4.0
3394103\H,3.3502101221,3.2315342488,2.2430578646\H,4.3701115327,-0.344
4470622,2.1588370168\H,3.2368852539,-0.8522099528,0.8962480049\C,1.317
515819,-1.0707296185,-0.7464704881\H,2.1601971241,-1.7544559063,-0.610
8308662\H,1.469614117,2.2427369105,0.1032521217\H,0.1591159934,0.88459
16004,1.8235888739\C,0.4531512485,-1.6848464218,-1.8201930221\O,-0.032
5857378,-1.1196112595,-2.7695930581\O,0.2350479828,-2.9965931269,-1.58
045196\H,-0.3527650078,-3.3234354297,-2.2787783056\Version=ES64L-G09R
evE.01\State=1-A\HF=-577.7461071\RMSD=4.261e-09\RMSF=2.974e-06\Dipole=
0.158791,-0.2947371,0.472049\Quadrupole=0.048854,4.3339041,-4.3827581,
1.8637629,-4.0802816,2.1595185\PG=C01 [X(C11H14O2)]\@\

7c(iii) [transition state]

1\1\GINC-R2470\FTS\RM062X\6-31+G(d,p)\C12H19N1\ROOT\07-Aug-2017\0\#\#M0
62X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,n
oeigentest,maxcyc=200) maxdisk=1610612736\|a1\|0,1\C,1.4201053655,0.98
73321064,0.1270830437\C,0.7594141956,0.2524321832,1.1062161099\C,1.703
8864622,0.1209650586,-1.0853178476\C,0.5395242754,-1.1744050106,0.6405
618211\H,2.721791861,0.2277682998,-1.479559593\H,1.0102664051,0.399125
8521,-1.8903696191\H,0.7813136585,-1.9310586323,1.3968567002\H,-0.5189
876933,-1.3023159815,0.3763997166\C,3.396424368,1.370368327,1.09898831
34\C,2.3015905843,0.1530017085,2.7214928712\C,2.3064303447,1.497701297
6,3.0945761007\C,2.9739134941,2.2398789682,2.1054092471\C,3.386975712,

-0.0109297885, 1.6935700468\H, 4.0243683695, 1.6558871967, 0.2610070654\H, 1.9426118468, -0.6588483483, 3.3460581777\H, 1.757205049, 1.9186662864, 3.9291410034\H, 3.0193545336, 3.3220587384, 2.058707948\H, 4.3388383701, -0.1493891953, 2.2319640056\H, 3.272604161, -0.8378551337, 0.9960230907\C, 1.3889655272, -1.328165473, -0.6436198586\H, 2.3330834809, -1.8561952482, -0.4030508201\H, 1.2618859738, 2.0493020133, -0.0111569834\H, 0.0472375988, 0.6982835734, 1.7888172367\N, 0.6973801581, -2.0916044165, -1.683193405\C, 1.5096993617, -2.1809219219, -2.8876927801\H, 0.97332143, -2.757307832, -3.6461280941\H, 1.7060196111, -1.1868547489, -3.2943047345\H, 2.481427062, -2.6773035809, -2.6974857359\C, 0.3831828813, -3.4344477595, -1.2176734908\H, 1.2929634228, -3.9997853991, -0.9356801389\H, -0.2794588773, -3.3962351506, -0.3507870353\H, -0.1291789936, -3.9840279889, -2.011772362\Version=ES64L-G09RevE.01\State=1-A\HF=-523.1363571\RMSE=3.641e-09\RMSE=2.373e-06\Dipole=0.1066737, -0.2171876, -0.091079\Quadrupole=-2.3772229, 2.3069841, 0.0702388, -0.0984852, -3.410153, -0.2625462\PG=C01 [X(C12H19N1)]\@

7c(iv) [transition state]

1\1\GINC-R545\FTS\RM062X\6-31+G(d,p)\C12H20N1(1+)\ROOT\07-Aug-2017\0\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS, calcfc, noeigentest, maxcyc=200) maxdisk=1610612736\1\1\C, 1.5123177022, 0.6816075702, -0.0423139124\C, 0.8437212772, -0.040665912, 0.946563243\C, 2.1661444059, -0.2627073343, -1.0409149819\C, 0.9888065518, -1.537761539, 0.7085174427\H, 3.2575466549, -0.301220016, -0.9495296444\H, 1.9701458875, 0.0279330414, -2.0824335157\H, 1.6708581718, -2.0230208629, 1.4159420797\H, 0.0361927634, -2.0689360428, 0.8148484019\C, 3.2365403271, 1.5127349593, 1.086089934\C, 2.128603411, 0.3209638964, 2.7195673388\C, 1.8752620897, 1.6824647896, 2.9030745162\C, 2.548655302, 2.4070944984, 1.9095710075\C, 3.3512534722, 0.2244057351, 1.8509413632\H, 3.9284209456, 1.8101282451, 0.3040304383\H, 1.8225512483, -0.4562782778, 3.4131022103\H, 1.1735148954, 2.0984574713, 3.6163489185\H, 2.4494698066, 3.4716568099, 1.7331444106\H, 4.2331453111, 0.3002540177, 2.5047659876\H, 3.4648570341, -0.6883036883, 1.2615110846\C, 1.5813769974, -1.6501094522, -0.7089441124\H, 2.3174931606, -2.4532421416, -0.8033993921\H, 1.202858507, 1.665391021, -0.3681204318\H, -0.034948008, 0.3300303935, 1.4567524751\N, 0.5105162101, -2.0205871413, -1.739999506\C, 0.081846886, -3.4486037832, -1.6264017456\H, -0.6035244471, -3.6764876507, -2.4427999468\H, 0.9623060429, -4.0882712254, -1.6830076521\H, -0.4222918541, -3.5899170404, -0.6711492255\C, -0.6740608537, -1.104052638, -1.7606625191\H, -1.2066670523, -1.1998054392, -0.8154038365\H, -0.3352306627, -0.0776829395, -1.8884796375\H, -1.3200203043, -1.401723925, -2.5867574055\H, 0.9726681203, -1.9217167393, -2.6494303867\Version=ES64L-G09RevE.01\State=1-A\HF=-523.5194767\RMSE=9.163e-09\RMSE=3.669e-06\Dipole=-1.3681582, -2.2842025, -2.6052187\Quadrupole=-5.5749701, 2.4816053, 3.0933648, 6.1339787, 6.279788, 11.1762992\PG=C01 [X(C12H20N1)]\@

8c(ii) [transition state]

1\1\GINC-R555\FTS\RM062X\6-31+G(d,p)\C12H15O2(1-)\ROOT\07-Aug-2017\0\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS, calcfc, noeigentest, maxcyc=200) maxdisk=1610612736\1\1\C, 1.5870138717, 0.7780693695, 0.1573208131\C, 0.857560011, -0.0044109727, 1.0574138018\C, 2.2874817999, 0.1547881249, -1.0422632915\C, 1.6239829927, -1.1593428482, -1.4660121308\C, 1.5313650945, -2.1009307499, -0.266837157\C, 0.6548665284, -1.4948606454, 0.8370138507\H, 3.3521232846, -0.0302473825, -0.8270884223\H, 2.2313621497, 0.8543671503, -1.8800242822\H, 2.2523065595, -1.6278559488, -2.2381272799\H, 2.5413237508, -2.3220681229, 0.1119551692\H, 0.7693870349, -2.0581707878, 1.7736172456\H, -0.3850105669, -1.6227216361, 0.5112066278\C, 3.3103368271, 1.412978423, 1.4074949843\C, 2.1442279929, 0.0789827394, 2.8750122264\C, 1.9710506334, 1.4130849778, 3.2495303726\C, 2.6847377747, 2.2284120929, 2.3528992773\C, 3.3693551543, 0.0304525085, 2.0013186308\H, 4.0022250666, 1.7642655935, 0.6484079042\H, 1.7847643475, -0.7728983595, 3.4435074058\H, 1.2612270403, 1.7685970656, 3.9889773762\H, 2.6123225135, 3.3092882689, 2.2964613061\H, 4.2585063448, -0.0263481337, 2.6535360578\H, 3.4092601828, -0.7895578672, 1.2852051924\H, 1.0801205725, -3.0452268568, -0.5833891005\H, 1.2671512387, 1.8060599409, 0.0300604206\H, 0.041046557, 0.4851198089, 1.5802974356\C, 0.2301717533, -0.9175787937, -2.1551736843\O, 0.1384016121, 0.1340577643, -2.8294955662\O, -0.6217381224, -1.8232747233, -1.9876951835\Version=ES64L-G09RevE.01\State=1-A\HF=-616.4893974\RMSE=7.165e-09\RMSE=3.661e-06\Dipole=2.7532634, 0.7947352, 3.7566317\Quadrupole=2.3

704141,10.6040874,-12.9745015,-7.5513454,-20.7527445,-6.3823516\PG=C01
[X(C12H15O2)]\@

8c(i) [transition state]

1\1\GINC-R664\FTS\RM062X\6-31+G(d,p)\C12H16O2\ROOT\07-Aug-2017\0\#M06
2X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,no
eigentest,maxcyc=200) maxdisk=1610612736\|a3\|0,1\C,1.459408602,1.0077
562571,0.3514445101\C,0.7718217042,0.2165008108,1.27753839\C,1.8279565
968,0.4944048261,-1.0311496233\C,1.6354880128,-1.0134791042,-1.2174154
869\C,0.3366228017,-1.4862158456,-0.5425457138\C,0.4318390208,-1.23377
16561,0.964019838\H,2.8511765677,0.7700603136,-1.3117888343\H,1.179637
1797,0.9971223015,-1.7596803888\H,2.4645227021,-1.582318975,-0.7781165
364\H,0.1716915519,-2.5487873012,-0.7460679094\H,1.1798951675,-1.92474
1514,1.3778687156\H,-0.5170688698,-1.4923484779,1.4445964484\C,3.41756
52814,1.2552748468,1.3400433893\C,2.2768357403,-0.0110613508,2.8859156
859\C,2.3535377841,1.3044214841,3.3517261546\C,3.048523977,2.076469132
9,2.4095054444\C,3.3526163544,-0.1607311342,1.8453219747\H,4.061534964
,1.5685652903,0.5245042666\H,1.8834815122,-0.8433626107,3.4614622046\H
,1.8317851452,1.6926423057,4.2190632367\H,3.1464987068,3.1558919643,2.
4322787531\H,4.2987584258,-0.383121681,2.364110974\H,3.1883561399,-0.9
331367048,1.0942276668\H,-0.5065141203,-0.92474756,-0.9651956099\H,1.2
715417517,2.0754037898,0.3786335391\H,0.0897921432,0.7191203452,1.9525
914091\C,1.6099283757,-1.3726450242,-2.6856735469\O,1.4299967724,-0.61
26896256,-3.6064146031\O,1.7882648712,-2.6980078342,-2.8777083292\H,1.
7253471376,-2.8610632686,-3.8313690191\Version=ES64L-G09RevE.01\State
=1-A\HF=-617.0454092\RMSD=5.751e-09\RMSF=2.596e-06\Dipole=-0.0521294,-
0.4565167,0.4309051\Quadrupole=0.3661229,3.1961292,-3.5622521,0.430130
3,-3.2155058,3.9685491\PG=C01 [X(C12H16O2)]\@

8c(iii) [transition state]

1\1\GINC-R732\FTS\RM062X\6-31+G(d,p)\C13H21N1\ROOT\07-Aug-2017\0\#M06
2X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,no
eigentest,maxcyc=200) maxdisk=1610612736\|a1\|0,1\C,1.3283216887,0.864
5388024,0.2115819769\C,0.6947861974,0.1710324526,1.2456856697\C,1.7103
014008,0.1894091833,-1.0970123792\C,1.5078230562,-1.3375290592,-1.1603
140065\C,0.2558326992,-1.7220627977,-0.372277154\C,0.4057683468,-1.312
2271867,1.0951636\H,2.7422359102,0.4376269163,-1.3676000014\H,1.074400
6862,0.6148400813,-1.8869736349\H,2.3751508812,-1.8440663869,-0.681179
1467\H,0.0823460413,-2.800359073,-0.4165012778\H,1.2013182023,-1.92649
46718,1.5408456999\H,-0.5081108146,-1.5600267837,1.6444426547\C,3.2892
871991,1.3232080624,1.1264108171\C,2.2402394232,0.1680343787,2.8158227
014\C,2.2670029305,1.5255420346,3.1493834767\C,2.9045349634,2.23012663
5,2.1179876293\C,3.3005355115,-0.0377126455,1.7679319628\H,3.898257356
2,1.5819193408,0.265964281\H,1.8992570256,-0.6193793071,3.4810195102\H
,1.7440464778,1.9745840479,3.9862027169\H,2.9514527079,3.309789772,2.0
314150837\H,4.2661113084,-0.1674343612,2.2826394013\H,3.1550763107,-0.
8848498593,1.0968936475\H,-0.6113826996,-1.223983626,-0.8253894011\H,1.
.0997491192,1.9191668541,0.1036699811\H,0.0075237822,0.7251722334,1.87
37953477\N,1.4326942161,-1.7683169448,-2.5637885268\C,2.6259363955,-1.
3864876266,-3.3078623403\H,2.5560916091,-1.7815972892,-4.3240931734\H,
2.7118352631,-0.3017229563,-3.3822709656\H,3.5525209108,-1.7812568465,
-2.8466550746\C,1.232430497,-3.2055809045,-2.6901393625\H,1.9983447616
,-3.7879563273,-2.1417541354\H,0.2464856846,-3.4990863461,-2.328583281
2\H,1.2886149503,-3.480599795,-3.7460722964\Version=ES64L-G09RevE.01\
State=1-A\HF=-562.4328933\RMSD=5.670e-09\RMSF=3.900e-06\Dipole=0.07200
26,-0.228637,-0.0390338\Quadrupole=-1.5469468,2.2575396,-0.7105927,-0.
1901799,-4.1003639,-0.1950986\PG=C01 [X(C13H21N1)]\@

8c(iv) [transition state]

1\1\GINC-R805\FTS\RM062X\6-31+G(d,p)\C13H22N1(1+)\ROOT\07-Aug-2017\0\
#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc
c,noeigentest,maxcyc=200) maxdisk=1610612736\|a3\|1,1\C,1.3587823755,0
.8766599534,0.1942946149\C,0.6651579874,0.2425915542,1.2296523341\C,1.
6505720745,0.1694007691,-1.1220949128\C,1.3406952244,-1.3281189663,-1.
0852439619\C,0.0443769541,-1.6301207586,-0.3512856843\C,0.2441019864,-
1.2149024132,1.1141905773\H,2.6920823589,0.314294437,-1.4417935026\H,1.
.0207379473,0.6417810708,-1.8900519212\H,2.1592435796,-1.8698582289,-0

.5996231189\H,-0.2147297086,-2.6937097621,-0.4090543427\H,0.9764362146
,-1.8951689321,1.5694965814\H,-0.6912432781,-1.3695355745,1.6573618045
\C,3.3696932305,1.1424524225,1.0912695237\C,2.2071563478,0.137990706,2
.8071307525\C,2.3531885092,1.4981147354,3.095556597\C,3.0611326101,2.1
092348334,2.0526534264\C,3.2490031539,-0.1922683065,1.7749165686\H,4.0
173243821,1.3240923595,0.2386938643\H,1.7984194942,-0.5912483588,3.499
5983568\H,1.8836381813,2.0156909343,3.9237214814\H,3.2241453094,3.1750
15775,1.944075084\H,4.1941184345,-0.3914978996,2.3023657291\H,3.038107
0673,-1.0526455849,1.1374941823\H,-0.7791295989,-1.0485157845,-0.78118
16823\H,1.224155401,1.9444415946,0.0748990153\H,0.0256079657,0.8585289
67,1.84833841\N,1.3514908187,-1.8722419335,-2.5201335576\C,1.710095707
7,-3.3232897672,-2.5698935096\H,1.7136172417,-3.6534933473,-3.60874204
68\H,2.6961087294,-3.4602674752,-2.1271395844\H,0.964111152,-3.8825370
259,-2.0053174996\C,0.0894150109,-1.6175162179,-3.2837707573\H,-0.6940
581777,-2.2573039531,-2.879569416\H,-0.1924019759,-0.57043181,-3.18618
64476\H,0.2658782116,-1.8613435576,-4.3313016452\H,2.0993300774,-1.359
6694548,-2.9997183128\Version=ES64L-G09RevE.01\State=1-A\HF=-562.8173
324\RMSD=4.023e-09\RMSF=4.133e-06\Dipole=-0.5402049,-2.1121594,-3.4514
264\Quadrupole=-11.1113261,-1.0915487,12.2028748,1.9156043,1.8864619,1
3.752845\PG=C01 [X(C13H22N1)]\@

7d(ii) [transition state]

1\1\GINC-R1208\FTS\RM062X\6-31+G(d,p)\C11H13O2(1-)\ROOT\07-Aug-2017\0\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,oeigentest,maxcyc=200) maxdisk=1610612736\|a6\|-1,1\C,1.9545815799
.0.9140906886,0.6118202311\C,1.2437072372,0.1451056137,1.5333058227\C,
2.2079523798,0.1256104384,-0.6638521726\C,0.9885379661,-1.2513470121,0
.9910423895\C,0.4532033953,2.4505000952,0.0432553301\C,-0.7433567027,1
.1304681778,1.4959698229\C,-0.4077499297,2.321521007,2.1471778583\C,0.
3268560415,3.12757126,1.2596808268\C,-0.6109769296,1.3895768266,0.0208
655493\H,3.2899705128,-0.0307308087,-0.7776105513\H,1.8557592996,0.616
7650179,-1.5783105054\H,1.5754622431,-1.9694632716,1.5811332257\H,-0.0
541336745,-1.5827154373,1.0414991868\H,-0.5385626451,2.5161413875,3.20
70507219\H,0.84787511,4.0409694506,1.5289448554\H,-0.4267681129,0.5380
10804,-0.6306518428\H,-1.5485075985,1.8644389081,-0.3169869441\H,0.889
8339361,2.867119375,-0.8589632501\H,-1.3873785495,0.3586517129,1.90540
49272\C,1.453669874,-1.2140685142,-0.4868599594\H,2.1339839186,-2.0532
499443,-0.6757081817\H,2.6469135529,1.6906622866,0.9177204471\H,1.3326
622525,0.2999033599,2.6031523859\C,0.2855037039,-1.4587543743,-1.50970
79317\O,-0.5434763254,-2.33159414,-1.1622326453\O,0.3182964647,-0.7835
909077,-2.5659775964\Version=ES64L-G09RevE.01\State=1-A\HF=-577.19147
97\RMSD=4.894e-09\RMSF=5.785e-06\Dipole=1.3374259,2.4775839,2.8963498\
Quadrupole=8.5395267,-4.6226739,-3.9168527,-4.5651992,-4.2413141,-11.9
36919\PG=C01 [X(C11H13O2)]\@

7d(i) [transition state]

1\1\GINC-R1494\FTS\RM062X\6-31+G(d,p)\C11H14O2\ROOT\07-Aug-2017\0\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,oeigentest,maxcyc=200) maxdisk=1610612736\|a4\|0,1\C,1.8995189841,0.99
95426952,0.5150431311\C,1.352079367,0.1415572537,1.4673363074\C,2.0643
818621,0.3022400466,-0.8249471311\C,1.0752002879,-1.2321185394,0.874088
0157\C,0.2156020621,2.3940587789,0.1421917192\C,-0.6740649007,0.985132
5402,1.7291130417\C,-0.3550260883,2.2018283889,2.3370196739\C,0.186696
9593,3.061363166,1.369003088\C,-0.7490147956,1.2452683346,0.2498525845
\H,3.0906814676,0.3794113378,-1.194753016\H,1.4219327024,0.7287180174,
-1.6066875282\H,1.5403510511,-2.018756295,1.4762899299\H,0.0066948328,
-1.467571854,0.8138157855\H,-0.3802984266,2.3952524303,3.4034830467\H,
0.6456829489,4.0227026011,1.5703879996\H,-0.5755183048,0.387016345,-0.
4011993484\H,-1.7571472758,1.6305226212,0.0278878317\H,0.4925948169,2.
855892181,-0.8005990468\H,-1.2031936629,0.1729693975,2.2176261933\C,1.
696823818,-1.1896187383,-0.5380768677\H,2.6165237221,-1.7809066337,-0.
5686094482\H,2.5685718416,1.8091999948,0.7757885246\H,1.5707751512,0.2
3228571,2.5232043391\C,0.7961408883,-1.723325018,-1.6227348049\O,-0.39
9180631,-1.8877092568,-1.5520957615\O,1.4820462623,-1.9648207723,-2.76
00786097\H,0.8418460597,-2.2584777328,-3.4265986491\Version=ES64L-G09
RevE.01\State=1-A\HF=-577.7459995\RMSD=5.843e-09\RMSF=3.311e-06\Dipole=
=0.6162676,0.0574148,-0.0869816\Quadrupole=-3.8189015,-0.5884373,4.407

3388,-0.2140232,0.0194543,0.3741792\PG=C01 [X(C11H14O2)]\@

7d(iii) [transition state]

1\1\GINC-R1514\FTS\RM062X\6-31+G(d,p)\C12H19N1\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc, noeigentest,maxcyc=200) maxdisk=1610612736\|a3\|0,1\C,1.7385260261,0.8615487948,0.4072491937\C,1.122223231,0.0454951033,1.358373439\C,1.8220690009,0.1485193567,-0.932925304\C,0.7337961416,-1.2898749095,0.7438078922\C,0.1928489598,2.4281700198,0.084548745\C,-0.8234936907,1.0866113047,1.6590566786\C,-0.3756009755,2.2522877481,2.2828707032\C,0.2432178445,3.0703627254,1.3231003812\C,-0.8806219814,1.3800473191,0.1856750332\H,2.8014077624,0.2673345119,-1.4057042335\H,1.0853099257,0.5255683789,-1.6525269618\H,0.9822179645,-2.1266879351,1.4048459023\H,-0.343532859,-1.3626651093,0.5409375475\H,-0.3697332794,2.4277398588,3.3526676713\H,0.8008150209,3.9750791074,1.537255929\H,-0.782781731,0.5213930782,-0.4798769719\H,-1.8477856109,1.8629075325,-0.0275834134\H,0.5056603545,2.8733676933,-0.8547063788\H,-1.4253630188,0.3212391705,2.1387749072\C,1.5624790394,-1.3316444888,-0.5734447469\H,2.5398185741,-1.75508961,-0.3077489882\H,2.4793753047,1.604022979,0.6733014823\H,1.3523047031,0.1099179436,2.413903201\N,1.0683039185,-2.151683672,-1.6734909076\C,1.1219912046,-3.5677691071,-1.3517903893\H,0.8903892493,-4.1555852159,-2.2450881166\H,2.1295792525,-3.8332921828,-1.0189171804\H,0.4068220158,-3.8570641658,-0.5594401572\C,-0.2487893954,-1.7993834128,-2.1742027515\H,-0.2833749048,-0.7499043162,-2.4742155001\H,-0.4599571791,-2.4028993167,-3.0619720035\H,-1.0605968678,-1.980665184,-1.4460347021\|Version=ES64L-G09RevE.01\State=1-A\HF=-523.1331171\RMSD=8.167e-09\RMSF=7.910e-06\Dipole=-0.0925524,-0.1850413,0.1222884\Quadrupole=-0.8531673,0.8677877,-0.0146204,2.4143861,1.9771929,-0.9677471\PG=C01 [X(C12H19N1)]\@

7d(iv) [transition state]

1\1\GINC-R1515\FTS\RM062X\6-31+G(d,p)\C12H20N1(1+)\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc, noeigentest,maxcyc=200) maxdisk=1610612736\|a1\|1,1\C,1.7961130172,0.8931138888,0.448079854\C,1.1785263655,0.0622937762,1.383496818\C,1.9326493666,0.1791085424,-0.8882512401\C,0.8448943938,-1.2843536634,0.759365059\C,0.2150849272,2.4292191246,0.0872667047\C,-0.806603937,1.0540529584,1.6355524297\C,-0.3808028634,2.2189168849,2.2756333529\C,0.2401239968,3.054599081,1.33471527\C,-0.8378891419,1.360357343,0.1650027344\H,2.9052772258,0.3572064832,-1.3548320071\H,1.1634139289,0.4920261237,-1.6134724905\H,1.0655883162,-2.1178266053,1.4316984763\H,-0.218291931,-1.3669038265,0.4793740753\H,-0.4106405743,2.3922985599,3.3447886731\H,0.7650067461,3.9745410649,1.5632982723\H,-0.7222339601,0.5109844593,-0.5131202548\H,-1.8088084475,1.8255689217,-0.0624816006\H,0.5277172535,2.8988658867,-0.8401740006\H,-1.4143469755,0.2852951377,2.102581337\C,1.7420061532,-1.2943275896,-0.4900412175\H,2.7100459406,-1.7510885069,-0.2566510222\H,2.5221045417,1.6467349764,0.7171307186\H,1.3827824029,0.1133982669,2.443244795\N,1.1729645826,-2.1389477895,-1.6159740417\C,2.0291772044,-2.088390493,-2.8408219817\H,1.5760347146,-2.7057474138,-3.6163369927\H,2.1116051242,-1.0575579447,-3.1804663507\H,3.0144082344,-2.4780317351,-2.5801036067\C,0.9402457956,-3.5536758506,-1.1913373107\H,0.2458251439,-3.5686814319,-0.3532903152\H,0.5293781703,-4.1133778786,-2.0314627306\H,1.8997032922,-3.9782719459,-0.8919497327\H,0.2620441757,-1.7289950525,-1.8531680654\|Version=ES64L-G09RevE.01\State=1-A\HF=-523.5195267\RMSD=5.398e-09\RMSF=5.431e-06\Dipole=0.6244408,-2.8682565,-2.1354594\Quadrupole=-10.1103846,8.5029432,1.6074414,-1.9162754,-3.8186161,12.4196868\PG=C01 [X(C12H20N1)]\@

8d(ii) [transition state]

1\1\GINC-R1530\FTS\RM062X\6-31+G(d,p)\C12H15O2(1-)\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc, noeigentest,maxcyc=200) maxdisk=1610612736\|a1\|-1,1\C,1.8362654204,0.7954400654,0.7478745989\C,1.08651665,-0.035905989,1.5913538473\C,2.4811927546,0.2804568815,-0.5306356124\C,1.8863116533,-1.0297305693,-1.0539143595\C,1.6559816433,-2.0097500998,0.097723932\C,0.6859094927,-1.4320933038,1.1381821507\C,0.304308807,2.1890515634,0.0331368154\C,-0.8521829763,1.0586084298,1.6659497957\C,-0.4468709411,2.2958782536,2.183

3972432\C,0.2537062808,2.9897596265,1.1841588553\C,-0.8004254583,1.180
3278733,0.1694595794\H,3.5455338203,0.122284864,-0.2885696553\H,2.4388
044122,1.0193407911,-1.3356558238\H,2.6228402549,-1.4675692352,-1.7438
055047\H,2.6200499466,-2.2311240438,0.583259188\H,0.6361385929,-2.0891
429585,2.0162405007\H,-0.3100658701,-1.4420750485,0.6804691672\H,-0.51
64789783,2.5968528954,3.2242004132\H,0.8179663225,3.904611076,1.337350
0228\H,-0.7034879224,0.2617503944,-0.4035492369\H,-1.7289953802,1.6750
088932,-0.1642600455\H,0.690871131,2.4842364668,-0.936932708\H,-1.4976
707121,0.3556822696,2.1854223049\H,1.2446124247,-2.9424141091,-0.29860
62442\H,2.4091441745,1.5807974468,1.2345191527\H,1.1901672072,0.108028
0061,2.6617752672\C,0.617091159,-0.7937395964,-1.9453269066\O,-0.29807
02986,-1.6463996344,-1.8438165881\O,0.6559163896,0.2244487908,-2.67633
01497\Version=ES64L-G09RevE.01\State=1-A\HF=-616.4934612\RMSD=4.570e-
09\RMSF=2.086e-05\Dipole=1.076444,1.0060757,3.1153234\Quadrupole=7.179
2173,1.4819838,-8.6612012,-0.7242497,-4.1393309,-6.5873869\PG=C01 [X(C
12H15O2)]\@

8d(i) [transition state]

1\1\GINC-R1819\FTS\RM062X\6-31+G(d,p)\C12H16O2\ROOT\07-Aug-2017\0\#M0
62X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,n
oeigentest,maxcyc=200) maxdisk=1610612736\@a6\0,1\C,1.7177648471,0.96
23648673,0.4886430343\C,1.2480670929,0.1082241311,1.4924080409\C,1.837
2612089,0.4939417853,-0.953963646\C,2.0197237169,-1.022703209,-1.03669
14439\C,0.8818378837,-1.7218082678,-0.2752046341\C,0.9274306996,-1.351
8059685,1.2120358964\C,0.0661865436,2.4289885097,0.3354531398\C,-0.722
1846677,0.9885992887,1.9472873739\C,-0.3174051645,2.1760082525,2.56477
58076\C,0.1636655876,3.053299925,1.5821118448\C,-0.9275299585,1.311009
0273,0.4917299869\H,2.6808395556,0.9997220053,-1.4342280933\H,0.956022
1764,0.7515937015,-1.5547122698\H,2.9724543505,-1.3212528598,-0.579959
7005\H,0.9610866959,-2.8078496757,-0.3845227665\H,1.718138568,-1.95056
93957,1.6854990043\H,-0.0078146873,-1.6622138521,1.6921064655\H,-0.242
751433,2.3309712381,3.6352081647\H,0.665847272,3.9949047384,1.77306490
78\H,-0.8263035943,0.4804218121,-0.2059758108\H,-1.9369674212,1.736535
6048,0.3744964428\H,0.2718352295,2.9153061474,-0.6130325211\H,-1.23767
86096,0.1813169746,2.4579101608\H,-0.0715860418,-1.4236133801,-0.72815
35055\H,2.4140031572,1.7388789211,0.7813215879\H,1.604247433,0.2907263
393,2.5004978733\C,2.0347609331,-1.4962571735,-2.4693100197\O,1.634623
7009,-0.8782510088,-3.426834117\O,2.5330323974,-2.7468507282,-2.582414
1008\H,2.4807225279,-2.9937697503,-3.5186041024\Version=ES64L-G09RevE
.01\State=1-A\HF=-617.0458424\RMSD=7.627e-09\RMSF=3.938e-06\Dipole=0.1
629522,-0.4419002,0.5071293\Quadrupole=-0.2438008,2.5263739,-2.2825731
,1.6166641,-0.577871,2.3735886\PG=C01 [X(C12H16O2)]\@

8d(iii) [transition state]

1\1\GINC-R721\FTS\RM062X\6-31+G(d,p)\C13H21N1\ROOT\07-Aug-2017\0\#M06
2X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,no
eigentest,maxcyc=200) maxdisk=1610612736\@a6\0,1\C,1.5153852033,0.860
2068389,0.2229691121\C,1.2022195251,0.1697222745,1.3899387209\C,1.4427
460997,0.0786357307,-1.0698121571\C,2.2662124702,-1.2220752465,-0.9408
146461\C,1.8564282632,-2.0133727559,0.3313255063\C,0.8196125798,-1.280
64515,1.2089131789\C,-0.2043031047,2.296801503,0.0607841256\C,-0.72286
74993,1.1471941653,1.9931550853\C,-0.2316102075,2.4079321552,2.3358228
252\C,0.0846745043,3.1078996183,1.1591329984\C,-1.1358887173,1.2240230
635,0.5499524431\H,1.8201913918,0.6924558351,-1.8909811929\H,0.4106142
1,-0.2017384898,-1.3240366033\H,3.3266906312,-0.9096345248,-0.84147372
2\H,2.7436691715,-2.2308423356,0.9355338883\H,0.7226283859,-1.78791256
88,2.1734429975\H,-0.1586845876,-1.362186995,0.7188130361\H,0.00434304
56,2.7357775849,3.3418814267\H,0.6033753014,4.0588963755,1.1164033744\H,
-1.1299707179,0.2873835515,-0.0069344731\H,-2.1613487664,1.625986472
0,0.5147367618\H,-0.1553086172,2.6172716619,-0.9750531256\H,-1.14283510
55,0.4349912603,2.6963798337\H,1.4285141748,-2.9716309184,0.0204239172
\H,2.2290745726,1.6751696963,0.2567891064\H,1.673903139,0.4502600153,2
.3245138926\N,2.137309821,-2.0828776345,-2.1264723771\C,3.1119386488,-
3.164822561,-2.0725347891\H,2.964084992,-3.834778604,-2.9237572559\H,4
.1514665898,-2.784939894,-2.104458585\H,2.9942736903,-3.7494019332,-1.
1583394509\C,2.3090876104,-1.3612592052,-3.3789226766\H,1.4897757988,-
0.6596553518,-3.5424722266\H,3.2662905751,-0.8054309269,-3.4195121545\

H,2.300326928,-2.0791397066,-4.2031897948\\Version=ES64L-G09RevE.01\\State=1-A\\HF=-562.4312088\\RMSD=3.971e-09\\RMSF=2.607e-06\\Dipole=0.2314039,-0.0753527,-0.0616594\\Quadrupole=-1.3252463,-0.8934095,2.2186558,0.8470225,-0.2469656,-1.4787348\\PG=C01 [X(C13H21N1)]\\@

8d(iv) [transition state]

1\\1\\GINC-R1076\\FTS\\RM062X\\6-31+G(d,p)\\C13H22N1(1+)\\ROOT\\07-Aug-2017\\0\\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,oeigentest,maxcyc=200) maxdisk=1610612736\\a4\\1,1\\C,1.6462761188,0.9258173011,0.1917989471\\C,1.4308718668,0.3333857166,1.4410053246\\C,1.7695829997,0.0751208926,-1.0664898049\\C,2.2753375488,-1.3171750163,-0.7006494949\\C,1.3554983052,-1.9751734645,0.3165660338\\C,1.425744521,-1.1761662596,1.6283301574\\C,-0.3011778219,1.9553119078,-0.1606874158\\C,-0.639095339,0.9171142092,1.8668971139\\C,-0.4507774845,2.2858960147,2.0850445298\\C,-0.2435715424,2.9167542494,0.8516787733\\C,-1.014719107,0.7658078103,0.4175214884\\H,2.4663614539,0.5625727693,-1.7596285313\\H,0.8072220028,-0.0157898614,-1.5900649925\\H,3.2877569618,-1.2363002424,-0.2884020113\\H,1.6400756659,-3.0140693772,0.5176099087\\H,2.35673624,-1.4490135497,2.1424333086\\H,0.6151300486,-1.5071798535,2.2844801222\\H,-0.347381509,2.7559975033,3.055978251\\H,0.0421028601,3.9531448839,0.7159297343\\H,-0.7978679851,-0.2009596423,-0.0394712329\\H,-2.0968967697,0.9445317804,0.3271236869\\H,-0.2819760403,2.1879387425,-1.2213841435\\H,-0.9437696408,0.217849292,2.6389917229\\H,0.3301987827,-1.9849950827,-0.0686796618\\H,2.1861370426,1.8624478199,0.1553432821\\H,1.8085907136,0.8678525818,2.304519621\\N,2.452892774,-2.1681668867,-1.9650509316\\C,1.1766269642,-2.7046842576,-2.5325278473\\H,1.3871203891,-3.1291539293,-3.5142060278\\H,0.7997675852,-3.4798206913,-1.8663053971\\H,0.4506115834,-1.8981589069,-2.6226120964\\C,3.4470441372,-3.2684021802,-1.7708988401\\H,4.4009944475,-2.8351439415,-1.4720914775\\H,3.0778746995,-3.9359142098,-0.9926448749\\H,3.5576813026,-3.8162482661,-2.7068539748\\H,2.8442302246,-1.5297508559,-2.6653832493\\Version=ES64L-G09RevE.01\\State=1-A\\HF=-562.8182939\\RMSD=4.533e-09\\RMSF=5.958e-06\\Dipole=1.8217186,-2.7889891,-2.4753439\\Quadrupole=-6.5937406,4.2670395,2.3267011,-8.7644083,-8.1756395,12.9917702\\PG=C01 [X(C13H22N1)]\\@

3a(ii) [product]

1\\1\\GINC-R852\\FTS\\RM062X\\6-31+G(d,p)\\C11H11O4(1-)\\ROOT\\07-Aug-2017\\0\\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,oeigentest,maxcyc=200) maxdisk=1610612736\\a3\\-1,1\\C,1.5370023521,0.4983366556,1.1471785717\\C,1.0337250016,1.1612756921,0.0288503028\\C,1.6293840173,-0.9857683339,0.8762929121\\C,0.8259946371,0.1637923578,-1.0999973258\\C,-0.2101688994,0.5897166721,2.7761823385\\C,-0.8698941145,1.861242503,0.5730599544\\C,-1.5899299785,0.6954672904,0.8422451109\\C,-1.2200160703,0.0265018555,1.9994362637\\H,1.3186174653,-1.6152449962,1.7175481173\\H,2.6700823961,-1.2468313883,0.6312752335\\H,-0.0719496289,0.3465213952,-1.7009936108\\H,1.6910924771,0.2059507752,-1.7757739367\\H,-2.2024525244,0.2422121139,0.0727584185\\H,-1.5780459299,-0.9770090006,2.2075814468\\H,0.2046200808,0.0772238402,3.6364069189\\H,-1.0694882992,2.4701327923,-0.3018044241\\O,-0.4456828095,2.649131708,1.6200157835\\C,-0.0032564218,2.0278379944,2.7584258727\\O,0.5139678429,2.7018024766,3.6259244468\\C,0.7978271282,-1.2126467338,-0.3966363176\\H,-0.23506223,-1.4730348285,-0.1509713179\\H,2.1571665837,0.9940478489,1.8896483839\\H,1.3220480664,2.192064804,-0.1684689856\\C,1.3487233662,-2.3216893268,-1.3512891304\\O,0.4818180469,-2.8715989602,-2.0678818293\\O,2.5899574446,-2.4935532069,-1.3253791978\\Version=ES64L-G09RevE.01\\State=1-A\\HF=-726.4238033\\RMSD=6.932e-09\\RMSF=2.918e-06\\Dipole=-1.9115079,2.9860418,2.178496\\Quadrupole=16.5295047,-12.7534986,-3.776006,10.6381758,7.9284177,-37.1086779\\PG=C01 [X(C11H11O4)]\\@

3a(i) [product]

1\\1\\GINC-R2470\\FTS\\RM062X\\6-31+G(d,p)\\C11H12O4\\ROOT\\07-Aug-2017\\0\\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,oeigentest,maxcyc=200) maxdisk=1610612736\\a4\\0,1\\C,1.5211533807,0.4639759746,1.2999536083\\C,1.1592476638,1.1401030929,0.1349251547\\C,1.6606302997,-1.0202335631,1.0276427824\\C,1.0702665993,0.1702627533,-1.0291940957\\C,-0.3047147434,0.5409596231,2.6902532627\\C,-0.8027387067,1.8937707927,0.4954461947\\C,-1.5468478743,0.7263430393,0.6760011528\\C,-1.28

04170369,0.0204914378,1.839489071\H,1.244122819,-1.6644794681,1.807101
8617\H,2.7233142264,-1.2759784411,0.9290456536\H,0.2332900794,0.351448
5523,-1.710041374\H,1.9932457336,0.2252288682,-1.6218791753\H,-2.14176
84095,0.3279184933,-0.137282826\H,-1.6916822794,-0.9695611437,2.011751
1056\H,0.0227986792,0.0075297839,3.57576915\H,-0.9221754295,2.52537587
98,-0.3780712299\O,-0.4333794957,2.6410074175,1.5835729735\C,-0.100840
4955,1.9873393827,2.7433203588\O,0.3449313538,2.6202753668,3.668817538
9\C,0.9623389146,-1.2088000378,-0.3271508667\H,-0.096380515,-1.4467059
787,-0.1882255098\H,2.0939654193,0.9359284364,2.0918876312\H,1.4760140
293,2.1652960967,-0.0316476317\C,1.5614445846,-2.304147947,-1.17074725
56\O,2.5941114862,-2.8892409292,-0.954090217\O,0.806736196,-2.55276853
75,-2.261994708\H,1.2578835209,-3.239854945,-2.7767056104\Version=ES6
4L-G09RevE.01\State=1-A\HF=-726.9698624\RMSD=3.479e-09\RMSF=4.491e-06\
Dipole=-0.6609645,-1.0689833,-1.6305151\Quadrupole=2.2892024,-3.701555
6,1.4123533,4.926506,1.1945602,-9.4144482\PG=C01 [X(C11H12O4)]\@

3a(iii) [product]

1\1\GINC-R2795\FTS\RM062X\6-31+G(d,p)\C12H17N1O2\ROOT\07-Aug-2017\0\#
M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc
,noeigentest,maxcyc=200) maxdisk=1610612736\|a6\|0,1\C,1.5140260182,0.
3969240142,1.2376370286\C,1.1335880604,1.0640030535,0.0736206036\C,1.6
156124808,-1.0905499026,0.9761888918\C,0.9937764969,0.0752356459,-1.06
69377099\C,-0.2703832441,0.53129371,2.6799728772\C,-0.7907035432,1.881
2999412,0.4894154659\C,-1.5646763935,0.7395398494,0.701760184\C,-1.285
0284002,0.0337637517,1.8620040722\H,1.2158742342,-1.7117045527,1.78363
13649\H,2.6747171305,-1.355203493,0.8423329409\H,0.1454595907,0.285093
6028,-1.727865941\H,1.9066624572,0.0865946411,-1.6785187672\H,-2.18980
09574,0.349192244,-0.0922699203\H,-1.7166819064,-0.944382214,2.0504869
005\H,0.0679319041,-0.0053367992,3.5594559607\H,-0.9170021962,2.510149
81,-0.3850291595\O,-0.3673310704,2.6259588177,1.5610617411\C,-0.021920
1106,1.9709383513,2.7152975267\O,0.4688871311,2.596936697,3.6234133509
\C,0.8849375536,-1.2950329092,-0.3670455099\H,-0.1838347583,-1.5069132
847,-0.1628959329\H,2.1193766048,0.8655130721,2.007319673\H,1.46639957
13,2.0800329735,-0.1164990455\N,1.4519592713,-2.3821093185,-1.15795076
1\C,1.3758459595,-3.6455867732,-0.4396048156\H,1.7972286807,-4.4413554
882,-1.0590419014\H,1.9552425094,-3.5957910806,0.4847157895\H,0.333386
2801,-3.9190644389,-0.1850315481\C,0.7736773812,-2.5046683614,-2.43957
30367\H,-0.3101774301,-2.6990079919,-2.3215395214\H,0.8991067911,-1.59
29084899,-3.0274492341\H,1.2105119035,-3.3324460774,-3.0039205669\Ver
sion=ES64L-G09RevE.01\State=1-A\HF=-672.3611177\RMSD=8.115e-09\RMSF=8.
614e-06\Dipole=-0.4200353,-1.5765805,-1.5142475\Quadrupole=3.7878344,-
2.0448745,-1.7429599,0.6140526,1.7392358,-11.226715\PG=C01 [X(C12H17N1
O2)]\@

3a(iv) [product]

1\1\GINC-R3168\FTS\RM062X\6-31+G(d,p)\C12H18N1O2(1+)\ROOT\07-Aug-2017\
0\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,ca
lcfc,noeigentest,maxcyc=200) maxdisk=1610612736\|a6\|1,1\C,1.495747391
6,0.412156428,1.213048373\C,1.1022487998,1.0839630871,0.0533425736\C,1
.6272986664,-1.0738783026,0.9375865299\C,0.9571917696,0.1073814985,-1.
0982175702\C,-0.2204006106,0.4969685393,2.6498024251\C,-0.8349183174,1.
.9057879577,0.5183255139\C,-1.5829657982,0.7430942656,0.7240687013\C,-
1.2671444277,0.0133182744,1.8593079816\H,1.2516131079,-1.7153626389,1.
7392806094\H,2.693286981,-1.3131081151,0.7907830277\H,0.0992804822,0.3
066711987,-1.7476182079\H,1.8633668775,0.141918796,-1.724681145\H,-2.2
644799085,0.3930917089,-0.042945212\H,-1.7126397033,-0.9565438653,2.06
16687145\H,0.1337548785,-0.0486503499,3.5184843503\H,-0.9964292181,2.5
527912666,-0.3375211435\O,-0.3677340924,2.6203194057,1.5817805293\C,0.
0059376124,1.946407849,2.7213903026\O,0.5136799534,2.547503966,3.62734
04285\C,0.8560153491,-1.248542222,-0.3808420196\H,-0.1886369028,-1.513
7376502,-0.1909659316\H,2.1304278606,0.8680961753,1.9654929654\H,1.425
7450709,2.0994202894,-0.1468584611\N,1.4031495624,-2.3842706119,-1.218
5246046\C,1.372704417,-3.6885384153,-0.4845658346\H,1.7760155396,-4.46
72591081,-1.1315272118\H,1.9703941863,-3.6068277079,0.4214671629\H,0.3
34434924,-3.91045891,-0.2335084516\C,0.6972003828,-2.50249414,-2.53303
00199\H,-0.3573640078,-2.6982748964,-2.3334095192\H,0.8097990508,-1.57
26907027,-3.0876459643\H,1.1316670393,-3.3295690949,-3.0941145776\H,2.

3860660836,-2.159244975,-1.4124173145\\Version=ES64L-G09RevE.01\\State=1-A\\HF=-672.7324298\\RMSD=3.882e-09\\RMSF=2.559e-06\\Dipole=0.9501378,-4.8009791,-4.0230186\\Quadrupole=-3.9224385,5.6905097,-1.7680712,-7.4312978,-4.2753038,3.7038895\\PG=C01 [X(C12H18N1O2)]\\@

5a(ii) [product]

1\\1\\GINC-R3200\\FTS\\RM062X\\6-31+G(d,p)\\C12H13O4(1-)-\\ROOT\\07-Aug-2017\\0\\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,oeigentest,maxcyc=200) maxdisk=2147483648\\a4\\0,1\\C,1.3194188109,-0.0495575418,1.0309073418\\C,1.1561618793,0.8622146426,-0.016201169\\C,0.7967154855,-1.4565721613,0.9351047702\\C,0.8392853752,-1.9729263258,-0.5054231523\\C,0.0811914412,-0.9925874051,-1.4033415176\\C,0.7867549323,0.364358106,-1.4076327608\\C,-0.3963519814,0.8179112179,2.799141957\\C,-0.3201383124,2.1118183355,0.4965686498\\C,-1.4731636355,1.3383364388,0.7319618778\\C,-1.4746521263,0.6494789971,1.9344030961\\H,-0.2486526271,-1.4860855311,1.2760519985\\H,1.387617698,-2.0965024935,1.5951600638\\H,0.3531429836,-2.9548222898,-0.5602558472\\H,-0.9536360314,-0.8787993908,-1.0459134204\\H,0.188101053,1.1135362296,-1.9448318579\\H,1.7280288865,0.2530540228,-1.9611937425\\H,-2.1841870295,1.1542150907,-0.0633759177\\H,-2.2349241468,-0.0957161389,2.1522184705\\H,-0.2833324716,0.2262574289,3.6997379954\\H,-0.2526305504,2.7492976554,-0.3795746673\\O,0.286190835,2.7303090823,1.5691903843\\C,0.4030694836,2.0206225236,2.7430591585\\O,1.1252072198,2.4658629102,3.6131852617\\H,0.0513858034,-1.3879654381,-2.4229143883\\H,2.0438905339,0.1802945146,1.8053915874\\H,1.8712456143,1.684581335,-0.0068297381\\C,2.3011870488,-2.1333379153,-1.0396622806\\O,2.3857319983,-2.6248745947,-2.1879692967\\O,3.2114408294,-1.7189573047,-0.2819128565\\Version=ES64L-G09RevE.01\\State=1-A\\HF=-765.7227208\\RMSD=7.831e-09\\RMSF=6.883e-06\\Dipole=-3.7949197,1.7966425,0.9146466\\Quadrupole=5.6392567,-3.4454579,-2.1937988,15.3341552,9.6422977,-28.4487321\\PG=C01 [X(C12H13O4)]\\@

5a(i) [product]

1\\1\\GINC-R3260\\FTS\\RM062X\\6-31+G(d,p)\\C12H14O4\\ROOT\\07-Aug-2017\\0\\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,oeigentest,maxcyc=200) maxdisk=2147483648\\a3\\0,1\\C,1.2311879528,-0.0346095773,0.9457445174\\C,1.0486774379,0.8183394297,-0.1534333176\\C,0.7334490576,-1.4669079867,0.9076756618\\C,0.7090278184,-2.0233001684,-0.5250406899\\C,-0.1054728645,-1.0849277442,-1.4160553851\\C,0.5347855954,0.3038892438,-1.4910866547\\C,-0.1740233468,0.7723465978,2.6234024078\\C,-0.3384489396,2.2298225676,0.4513502823\\C,-1.4691836032,1.4608019001,0.7589360158\\C,-1.3760746997,0.7062033218,1.9154994357\\H,-0.2972000597,-1.5289196495,1.2739211424\\H,1.3477313085,-2.0909566092,1.5606759896\\H,0.2400958389,-3.0164488519,-0.5011219911\\H,-1.1132642928,-1.0154485949,-0.9883437493\\H,-0.1730898695,1.0099115374,-1.9403616272\\H,1.390675799,0.2530736804,-2.1731068204\\H,-2.2687847726,1.3493906815,0.03645908\\H,-2.1349788403,-0.0233334198,2.1807047935\\H,0.0193605341,0.1336112549,3.4783809543\\H,-0.30994344,2.8807795818,-0.4161191765\\O,0.4121418484,2.761667286,1.4697777899\\C,0.6122263476,2.0000862498,2.5937444888\\O,1.4051874302,2.3736233178,3.4240166105\\H,-0.2003971834,-1.4960236432,-2.4246222552\\H,2.0603999777,0.1756430088,1.6149370222\\H,1.7785323773,1.6219249599,-0.2351387475\\C,2.0962529107,-2.2575130478,-1.0913766877\\O,2.4412478888,-2.0200182803,-2.2242015364\\O,2.931201456,-2.8176008486,-0.192913169\\H,3.7790813328,-2.9639661974,-0.6403433845\\Version=ES64L-G09RevE.01\\State=1-A\\HF=-766.2675683\\RMSD=5.321e-09\\RMSF=2.453e-06\\Dipole=-1.0603172,-1.3606056,-0.9717163\\Quadrupole=8.813829,-0.3577019,-8.4561271,-3.4819691,-0.8587463,-11.8054704\\PG=C01 [X(C12H14O4)]\\@

5a(iii) [product]

1\\1\\GINC-R3362\\FTS\\RM062X\\6-31+G(d,p)\\C13H19N1O2\\ROOT\\07-Aug-2017\\0\\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,oeigentest,maxcyc=200) maxdisk=2147483648\\a1\\0,1\\C,1.4820186434,0.2953355591,1.0830973745\\C,1.1914539803,1.2123786665,0.0616091358\\C,1.5811101079,-1.1931518353,0.8052005504\\C,0.9087596507,-1.5843712377,-0.5200683582\\C,1.4600064523,-0.6811051315,-1.6218485706\\C,0.9958405888,0.7589029557,-1.3829711519\\C,-0.3040160219,0.3023127356,2.4853619262\\C,-0.6392034892,2.1083264634,0.6250558533\\C,-1.5298442721,1.0301138489,0.5914553957\\C,-1.3421964719,0.0764688967,1.5766486312\\H,1.1805994979,-1

.7788386668,1.6387654048\H,2.6515677037,-1.4395800278,0.7422154225\H,-
0.1664378055,-1.369420204,-0.4348362867\H,1.1176338078,-1.0410818517,-
2.5973002378\H,-0.0592053503,0.8328122021,-1.673110017\H,1.5434890234,
1.4412208681,-2.0414026903\H,-2.1744685233,0.8765161385,-0.2651622509\
H,-1.8668704927,-0.8741702905,1.5613317266\H,-0.0383237465,-0.43094189
65,3.2388296361\H,-0.6823899107,2.9122785776,-0.1019615746\O,-0.197716
9834,2.5822404325,1.8365586613\C,0.0449933024,1.6779225579,2.835388891
\O,0.5398674196,2.056405553,3.8697072645\H,2.5570198304,-0.7145730508,
-1.6189188768\H,2.0866359797,0.6515418541,1.9142038392\H,1.6321575598,
2.1982310893,0.1886062804\N,0.9929182286,-3.0034335669,-0.8688252113\C
2.3423251524,-3.5220412956,-1.0188542478\H,2.287743607,-4.527637838,-
1.4462602761\H,2.9170705126,-2.8993205001,-1.7081614786\H,2.8954085592
,-3.5936364292,-0.0651493367\C,0.2106053202,-3.849952709,0.0139765117\
H,0.6366390155,-3.9453678772,1.0292398417\H,-0.8052772012,-3.452357177
5,0.1019730139\H,0.1455563251,-4.8550768129,-0.4136047956\Version=ES6
4L-G09RevE.01\State=1-A\HF=-711.6550846\RMSD=4.549e-09\RMSF=2.721e-06\
Dipole=-0.1200613,-1.127993,-1.6144533\Quadrupole=6.940256,0.5117526,-
7.4520085,-0.6264538,-0.4878639,-12.9039594\PG=C01 [X(C13H19N1O2)]\@

5a(iv) [product]

1\1\GINC-R2701\FTS\RM062X\6-31+G(d,p)\C13H20N1O2(1+)\ROOT\07-Aug-2017\
0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,ca
lcf,oeigentest,maxcyc=200) maxdisk=2147483648\la2\1,1\C,1.389731535
4,0.2432714975,1.1451948842\C,1.2328558935,1.1997135511,0.1294589661\C
1.4719961568,-1.2416341052,0.8253829748\C,0.8986279246,-1.535969116,-
0.5549625294\C,1.5411498292,-0.6423677754,-1.6050427262\C,1.0828798693
,0.7977246159,-1.3327989905\C,-0.4588748101,0.2825230667,2.3852732683\
C,-0.5609712481,2.237059326,0.6479370556\C,-1.5151953054,1.2257881218,
0.4865361483\C,-1.4633980065,0.1995191393,1.4124457726\H,0.9637549068,
-1.8422565577,1.5894729149\H,2.5342546878,-1.5225566435,0.849539111\H,
-0.1854113867,-1.3686456092,-0.5417506236\H,1.2568000006,-0.929834487,
-2.6230590233\H,0.0431858771,0.8924857456,-1.6653682489\H,1.6698277176
1.477251224,-1.9559556823\H,-2.1410482492,1.2012893533,-0.3974935722\
H,-2.0841485766,-0.6878627867,1.3254378013\H,-0.3125210211,-0.50519880
47,3.1175950654\H,-0.5053489991,3.0873790621,-0.0236450097\O,-0.141393
6789,2.587403677,1.9012916841\C,-0.0421877705,1.6094609042,2.857560374
4\O,0.4075181142,1.8729454348,3.9396607019\H,2.6327263933,-0.704528926
6,-1.5257634045\H,1.9743935223,0.5278907407,2.0155664116\H,1.734029272
9,2.1469872538,0.3044849286\N,1.0485262902,-3.025961883,-0.8706811445\
C,0.0491647889,-3.4918945033,-1.8822585959\H,0.1820071426,-4.561560372
5,-2.0443260171\H,-0.9539803634,-3.2886153678,-1.508887063\H,0.2205821
097,-2.9523633966,-2.8134342465\C,2.432784988,-3.4327517592,-1.2728363
74\H,2.641268282,-3.0223331114,-2.2601332903\H,3.1508180309,-3.0550823
383,-0.546864176\H,2.4748551374,-4.5213074417,-1.3064781007\H,0.837917
9446,-3.5147757281,0.0059757554\Version=ES64L-G09RevE.01\State=1-A\HF
=-712.0285873\RMSD=2.662e-09\RMSF=1.591e-06\Dipole=0.611671,-4.9017795
,-3.9586435\Quadrupole=-4.1984412,15.985783,-11.7873417,-5.5622815,-2.
4830767,3.0560329\PG=C01 [X(C13H20N1O2)]\@

3b(ii) [product]

1\1\GINC-R1109\FTS\RM062X\6-31+G(d,p)\C11H11O4(1-)\ROOT\07-Aug-2017\
0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calc
fc,oeigentest,maxcyc=200) maxdisk=1610612736\la4\1,1\C,0.9102263651
,0.3881213046,1.5551319403\C,0.7034226295,1.173516747,0.4183818411\C,0
.8014865042,-1.0846127074,1.2092947072\C,0.3556900352,0.2934252293,-0.
7712735983\H,-0.1321790998,-1.4671293524,1.6481274468\H,1.6219276262,-
1.7069123957,1.5789328025\H,-0.7262010568,0.3633651926,-0.9539107959\H
,0.8707491601,0.5573793105,-1.700637581\C,3.1553076717,0.6107135145,2.
0904521872\C,2.5493607911,2.088149147,0.015620954\C,3.401540619,1.0109
766606,-0.2370334403\C,3.7103843316,0.2293835495,0.8657305018\H,3.2601
772623,-0.0031303357,2.9781801875\H,2.2356430135,2.7704978363,-0.76695
96721\H,3.5604887862,0.6583689218,-1.2495790566\H,4.1720286201,-0.7441
83809,0.7401914724\O,2.6347505345,2.7535794942,1.2231827881\C,2.870646
0308,2.0126265463,2.3472395899\O,2.8033307956,2.5604678912,3.431798271
5\C,0.7625163383,-1.1298598718,-0.3338046849\H,0.0151972452,-1.8573055
236,-0.6729651595\H,0.6955427422,0.7481269774,2.5575720082\H,0.2772811
317,2.1695124882,0.5144470403\C,2.0968247983,-1.6388409479,-0.99067057

73\O,2.3324331465,-1.2099022078,-2.1447653485\O,2.7670479775,-2.447759
6596,-0.3076028245\Version=ES64L-G09RevE.01\State=1-A\HF=-726.4319623
\RMSD=7.816e-09\RMSF=2.268e-06\Dipole=-1.2775115,1.658995,0.8942732\Qu
adpole=14.8135268,-8.1340238,-6.679503,1.6752664,0.364026,-21.327731
4\PG=C01 [X(C11H11O4)]\@

3b(i) [product]

1\1\GINC-R1129\FTS\RM062X\6-31+G(d,p)\C11H12O4\ROOT\07-Aug-2017\0\#M0
62X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcf,n
oeigentest,maxcyc=200) maxdisk=1610612736\|a2\|0,1\C,0.8683465653,0.37
84813542,1.516737422\C,0.7217997886,1.2017627599,0.4005758736\C,0.6489
373943,-1.0748732488,1.1456466259\C,0.3579665682,0.3830447402,-0.82648
3079\H,-0.322006373,-1.3943421894,1.5415282013\H,1.3978488071,-1.76253
36946,1.5451065941\H,-0.7019215946,0.5311504626,-1.0605423272\H,0.9299
190522,0.6380256418,-1.7235679576\C,3.0809672031,0.4123304937,2.070227
8525\C,2.6395225438,2.0806505633,0.0942340469\C,3.422402027,0.96657122
52,-0.2125851435\C,3.6543621439,0.0924287959,0.8374976648\H,3.14358837
48,-0.2594510268,2.919364101\H,2.3882601599,2.8304703543,-0.6477273066
\H,3.6436319461,0.722408045,-1.243851945\H,4.1232926886,-0.8743630202,
0.6815112884\O,2.7084722254,2.6431945796,1.3434067305\C,2.8850033808,1
.8169513647,2.4229202188\O,2.8309834758,2.2812803056,3.5361300453\C,0.
6068377694,-1.0811741033,-0.4046651004\H,-0.2088779017,-1.7290859258,-
0.7484622997\H,0.6465788056,0.7192515185,2.5231089699\H,0.3436493472,2
.2136520386,0.5077964855\C,1.8249241958,-1.6872334203,-1.0714602576\O,
2.3478884916,-1.2933663491,-2.0864655667\O,2.2445658258,-2.8074052439,
-0.4471881111\H,2.9658740892,-3.1780040209,-0.979114026\Version=ES64L
-G09RevE.01\State=1-A\HF=-726.9697788\RMSD=6.758e-09\RMSF=2.043e-06\Di
pole=-0.7001483,-1.460689,-1.203593\Quadrupole=6.6244237,2.3571571,-8.
9815808,-4.2521379,-1.9485962,-8.969653\PG=C01 [X(C11H12O4)]\@

3b(iii) [product]

1\1\GINC-R1173\FTS\RM062X\6-31+G(d,p)\C12H17N1O2\ROOT\07-Aug-2017\0\#
M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcf
,noeigentest,maxcyc=200) maxdisk=1610612736\|a3\|0,1\C,0.9398441501,0.
346012036,1.4137178295\C,0.8475923476,1.1600861414,0.2817032273\C,0.97
75164729,-1.1070027277,0.986577868\C,0.7118729862,0.2962109018,-0.9629
66377\H,0.4724354543,-1.7629210697,1.7006814987\H,2.0110702104,-1.4620
701146,0.8660585333\H,-0.0287737328,0.6991213468,-1.6597770605\H,1.664
1168224,0.1962404176,-1.5004110505\C,3.0427437201,0.6796938362,2.30531
67912\C,2.6978298631,2.2095242161,0.1944211308\C,3.6241156238,1.173748
7018,0.057800077\C,3.8063000859,0.3777027875,1.1778516819\H,3.06231458
12,0.0545728891,3.1911036783\H,2.4851500954,2.9016451284,-0.61288653\H
,4.0246898202,0.9212600948,-0.9159511476\H,4.3990499346,-0.5304571,1.1
369124453\O,2.5361627246,2.8239066636,1.4105921886\C,2.6292280249,2.05
93937372,2.5458423044\O,2.3459450676,2.5525176326,3.6110562033\C,0.321
995721,-1.0898296016,-0.408223772\H,-0.7806176954,-1.1141472237,-0.274
9906909\H,0.5567409128,0.644628742,2.3835416733\H,0.3666485531,2.13139
65325,0.3385668869\N,0.7476218165,-2.1912884605,-1.2607706057\C,0.4248
670163,-3.4773773274,-0.6604651251\H,0.7425191733,-4.2801141031,-1.330
8293788\H,0.9546345777,-3.6005864294,0.2865610627\H,-0.6600354304,-3.5
913928855,-0.4725240645\C,0.1409608238,-2.0960577901,-2.5803101123\H,-
0.9648753943,-2.1174834342,-2.5350458914\H,0.4481296856,-1.172561836,-
3.0759713504\H,0.4750719875,-2.9357877017,-3.1951019236\Version=ES64L
-G09RevE.01\State=1-A\HF=-672.3577052\RMSD=8.334e-09\RMSF=7.871e-06\Di
pole=-0.274691,-1.4061723,-1.6902464\Quadrupole=4.6655909,-1.3206194,-
3.3449715,-1.5598141,-1.0216125,-11.2215274\PG=C01 [X(C12H17N1O2)]\@

3b(iv) [product]

1\1\GINC-R2267\FTS\RM062X\6-31+G(d,p)\C12H18N1O2(1+)\ROOT\07-Aug-2017\
0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,ca
lcf,oeigentest,maxcyc=200) maxdisk=1610612736\|a6\|1,1\C,1.207565276
7,0.1969632435,1.5757677927\C,0.764173854,0.962507529,0.4904993466\C,1
.3736554451,-1.2498168709,1.1423366255\C,0.552729585,0.0696781548,-0.7
22409517\H,1.1106310757,-1.9573716332,1.9317490748\H,2.411735144,-1.45
11194168,0.8304729694\H,-0.3365368469,0.3447526926,-1.2945247859\H,1.4
195266384,0.1030524724,-1.4019109647\C,3.2996136892,0.8422550005,2.052
7080933\C,2.3699105771,2.3660258583,0.115768502\C,3.4025276369,1.49070

15772,-0.2272011308\C,3.9035275074,0.7059559113,0.8003340096\H,3.59106
73502,0.2211232698,2.8934925659\H,1.9121250169,3.0318528689,-0.6080016
677\H,3.6903869978,1.3688384033,-1.2647109064\H,4.6433768945,-0.068179
8755,0.6204703934\O,2.3008636007,2.8960701122,1.3703064649\C,2.7325042
608,2.1410974179,2.4366356117\O,2.5741471775,2.549068973,3.5540056062\
C,0.4507532829,-1.3232379768,-0.0822431485\H,-0.5802957329,-1.54112697
91,0.216763502\H,0.9375163006,0.4272001099,2.6003270613\H,0.1330589872
,1.831193915,0.6381138247\N,0.8334797149,-2.4361296807,-1.0377315559\C
,0.8181715125,-3.7763184487,-0.3723867526\H,1.0895066217,-4.5374061193
,-1.1036959337\H,1.5293459384,-3.7775677695,0.4516934954\H,-0.19108550
31,-3.9579413552,0.000224231\C,-0.0259830032,-2.4414662548,-2.26235361
47\H,-1.0602693564,-2.5922353648,-1.9494599761\H,0.0759234324,-1.48824
82655,-2.7779828881\H,0.290282276,-3.2563865133,-2.9132010998\H,1.7979
416479,-2.2452899854,-1.3336052285\Version=ES64L-G09RevE.01\State=1-A
\HF=-672.7297494\RMSD=7.229e-09\RMSF=2.287e-06\Dipole=-1.4557789,-4.83
59546,-3.7958444\Quadrupole=-3.0946538,9.0393865,-5.9447328,5.9171837,
4.1502437,2.5232319\PG=C01 [X(C12H18N1O2)]\@

5c(ii) [product]

1\1\GINC-R2283\FTS\RM062X\6-31+G(d,p)\C12H13O4(1-)\ROOT\07-Aug-2017\0\
\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calc
fc,noeigentest,maxcyc=200) maxdisk=2147483648\la5\1,1\C,0.9030751874
,0.4458870225,1.3677142454\C,0.7865305847,1.2121752218,0.1962172956\C,
0.7007407215,-1.0578169898,1.3693803154\C,0.6840992526,-1.6963566353,-
0.0258173771\C,-0.1441466498,-0.8436240331,-0.9854225376\C,0.454847181
8,0.5578903464,-1.1405498348\H,-0.2746570602,-1.2242197948,1.855430382
3\H,1.4502238572,-1.5768612139,1.9731664464\H,0.2054208356,-2.67915750
49,0.0834343577\H,-1.1744256869,-0.7676853387,-0.602979503\H,-0.239603
2972,1.2103916132,-1.6854640548\H,1.3530286787,0.4401028669,-1.7534279
751\C,3.118005778,0.5887069024,1.9854345428\C,2.646333811,2.0947465863
,-0.0937958898\C,3.4940979884,1.004284467,-0.3175881215\C,3.7268332842
,0.2023694535,0.7857951248\H,3.1624066884,-0.0391296171,2.8683933939\H
,2.3874760139,2.7930322636,-0.8832255588\H,3.7072008882,0.6569975655,-
1.3209310117\H,4.1633102947,-0.7858226544,0.6808003597\O,2.7062641176,
2.7541466675,1.1201390159\C,2.8835413675,2.0002548149,2.2456981344\O,2
.8074750764,2.5449918415,3.3310921833\H,-0.1795538057,-1.3250176589,-1
.9673117616\H,0.6583185425,0.9411969409,2.3058702665\H,0.3942689676,2.
2165813859,0.346595226\C,2.1298118423,-2.0234068979,-0.5327205011\O,2.
8472676105,-2.6336446663,0.2973010164\O,2.426440929,-1.6602569549,-1.6
956281796\Version=ES64L-G09RevE.01\State=1-A\HF=-765.7295699\RMSD=6.5
75e-09\RMSF=3.414e-06\Dipole=-1.5704395,1.7294787,-0.0157813\Quadrupol
e=11.9668506,-10.8680694,-1.0987812,2.7505521,-1.1291529,-18.0430334\PG
G=C01 [X(C12H13O4)]\@

5c(i) [product]

1\1\GINC-R2293\FTS\RM062X\6-31+G(d,p)\C12H14O4\ROOT\07-Aug-2017\0\#M0
62X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,n
oeigentest,maxcyc=200) maxdisk=2147483648\la5\0,1\C,1.0310311244,0.27
30823964,1.2018420123\C,0.9431976194,1.1516973963,0.1198252801\C,1.292
5349121,-1.1665940853,0.854407463\C,0.2426926625,-1.6781444545,-0.1833
96018\C,-0.0358180439,-0.6438790653,-1.2941194527\C,0.9743313303,0.516
2704323,-1.2539085026\H,1.2937239512,-1.8119170442,1.7354833945\H,2.28
42283043,-1.2428668498,0.3870216316\H,-0.6752269297,-1.9194216151,0.36
11932494\H,-1.0427508893,-0.2368915797,-1.1611848773\H,0.7429934575,1.
2511171091,-2.0305778819\H,1.9730332217,0.1197508164,-1.4731525144\C,3
.0381728887,0.7572281159,2.2830935188\C,2.6534536301,2.3977457198,0.26
08342079\C,3.7004973366,1.4842299694,0.1217320244\C,3.9009964694,0.629
3735352,1.1951958339\H,3.0722998345,0.0714218462,3.1224142635\H,2.4170
679872,3.1239852714,-0.5092604938\H,4.1888866545,1.3556275287,-0.83637
54383\H,4.5968989644,-0.2015193327,1.136016562\O,2.3426132657,2.893056
6588,1.5015690201\C,2.4479935062,2.0582205451,2.5854976077\O,2.0398503
241,2.4337270543,3.6579019089\H,-0.0012667013,-1.1357496573,-2.2694529
347\H,0.523301011,0.5025985542,2.1342752155\H,0.3331660624,2.043215688
1,0.2469157996\C,0.7845628943,-2.9743569616,-0.74256871\O,1.2864920972
,-3.1266090195,-1.8302612615\O,0.7019810646,-3.9768049232,0.156727243\
H,1.10396099,-4.7621990491,-0.245722151\Version=ES64L-G09RevE.01\Stat
e=1-A\HF=-766.2664273\RMSD=5.301e-09\RMSF=6.378e-06\Dipole=0.0304683,-

1.0654048,-1.218429\Quadrupole=7.7496629,1.4176597,-9.1673227,-1.27517
07,0.0782631,-14.9718866\PG=C01 [X(C12H14O4)]\@

5c(iii) [product]

1\1\GINC-R2333\FTS\RM062X\6-31+G(d,p)\C13H19N1O2\ROOT\07-Aug-2017\0\#
M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc
,noeigentest,maxcyc=200) maxdisk=2147483648\la4\0,1\C,1.0614395958,0.
2676926406,1.2685225165\C,0.9497128516,1.1490952815,0.1910747858\C,1.2
031150474,-1.1868595421,0.9137474632\C,0.0722829621,-1.6576123586,-0.0
338651935\C,-0.2701460079,-0.5788256495,-1.1003362483\C,0.8121863599,0
.5112205815,-1.1769354162\H,1.2281974072,-1.8317914045,1.7949969227\H,
2.1595565731,-1.3190235759,0.3923860743\H,-0.8161099092,-1.8193513636,
0.5865166341\H,-1.2236754584,-0.1018608973,-0.8511160313\H,0.560527953
2,1.261114421,-1.9335201563\H,1.7623748528,0.0540130796,-1.4814224709\
C,3.1838753124,0.6393023522,2.1962287336\C,2.7497346114,2.2594153119,0
.1667148556\C,3.7188735679,1.272604092,-0.0299055067\C,3.9444820994,0.
428536545,1.0475060534\H,3.2346990911,-0.0322652186,3.0459150687\H,2.5
053326959,2.9857558614,-0.6009636868\H,4.1217462499,1.0918497668,-1.01
89212518\H,4.5750668863,-0.4504731445,0.9572049261\O,2.5770668349,2.80
20957112,1.4148273019\C,2.7047099195,1.9817263004,2.5081703642\O,2.402
8239194,2.4063490503,3.5977788474\H,-0.4079054011,-1.0502904866,-2.079
9792335\H,0.655022431,0.5416947363,2.2379120722\H,0.4186159662,2.08323
0197,0.3606078615\N,0.4081778128,-2.9818979634,-0.5726023536\C,-0.7641
22118,-3.6967430731,-1.0484920368\H,-0.4802558468,-4.7181900713,-1.318
5577056\H,-1.5138969209,-3.7494551926,-0.2544286591\H,-1.2293484859,-3
.2301449102,-1.9367643385\C,1.4453819613,-2.9844808972,-1.591223029\H,
1.1307637164,-2.511561863,-2.5396139547\H,2.3442097203,-2.4741286011,-
1.2373567482\H,1.7199307487,-4.0197767157,-1.8128194603\Version=ES64L
-G09RevE.01\State=1-A\HF=-711.6544905\RMSD=6.708e-09\RMSF=4.055e-06\Di
pole=-0.2057506,-1.1884185,-2.0011434\Quadrupole=7.1485312,-3.1217018,
-4.0268294,-2.271546,-2.4682348,-10.1607747\PG=C01 [X(C13H19N1O2)]\@

5c(iv) [product]

1\1\GINC-R2400\FTS\RM062X\6-31+G(d,p)\C13H20N1O2(1+)\ROOT\07-Aug-2017\
0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,ca
lcfc,noeigentest,maxcyc=200) maxdisk=2147483648\la3\1,1\C,1.048232090
1,0.2887315228,1.0921443664\C,1.0624019047,1.1593562937,-0.0012386411\
C,1.2612979129,-1.178798589,0.7834351831\C,0.2398256439,-1.5670194966,
-0.2967089576\C,0.3761701979,-0.6858818893,-1.5642554\C,1.3231374996,0
.5113613089,-1.3407247357\H,1.132004383,-1.7693829002,1.6924256891\H,2
.279703864,-1.3511740357,0.4038640182\H,-0.767099361,-1.4908639988,0.1
280813256\H,-0.6110883486,-0.3272161701,-1.8670480651\H,1.2100017623,1
.2213058079,-2.1633963068\H,2.3576883584,0.1495064757,-1.3747289128\C,
2.8949380516,0.6969735461,2.3079359965\C,2.6989348763,2.5007290661,0.4
026673381\C,3.7730064906,1.6138906087,0.3049871998\C,3.8798118853,0.67
27818008,1.3160582246\H,2.8738743682,-0.0401070204,3.1043688749\H,2.52
39105277,3.2795107716,-0.3316502717\H,4.3784026183,1.5923108059,-0.593
3239586\H,4.6120982743,-0.1276943676,1.2764817002\O,2.2247988415,2.877
437103,1.6273084265\C,2.2666110325,1.9752892693,2.6617152407\O,1.76155
43718,2.2553497082,3.7155484086\H,0.7636924213,-1.2803999061,-2.402883
3787\H,0.4262414981,0.5141955016,1.953722197\H,0.425630711,2.038389475
6,0.0330816399\N,0.3542608218,-3.0399919428,-0.696324973\C,0.465863292
2,-3.9747602978,0.4673018641\H,0.4106260105,-4.99809198,0.0966073933\H
,1.4136866786,-3.8161598892,0.9765729356\H,-0.3667275973,-3.7784051534
,1.1448132324\C,-0.7922688341,-3.4523188329,-1.5690367653\H,-1.6997072
867,-3.4188490536,-0.964427547\H,-0.8780455421,-2.7675730698,-2.410245
0744\H,-0.6187257067,-4.4671019218,-1.9263421436\H,1.2146542882,-3.128
3555511,-1.2480151232\Version=ES64L-G09RevE.01\State=1-A\HF=-712.0293
868\RMSD=3.457e-09\RMSF=5.456e-06\Dipole=-1.3229438,-5.242517,-3.51011
02\Quadrupole=-2.2360413,15.4642296,-13.2281884,13.0790163,5.4100832,-
0.6031589\PG=C01 [X(C13H20N1O2)]\@

5b(ii) [product]

1\1\GINC-R3365\FTS\RM062X\6-31+G(d,p)\C12H13O4(1-)\ROOT\07-Aug-2017\0\
\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calc
fc,noeigentest,maxcyc=200) maxdisk=2147483648\la2\1,1\C,1.3995649176

,0.2636882886,1.0262574993\C,1.0572363003,1.2054003753,0.0440780066\C,
1.4611985553,-1.2222302583,0.7010475479\C,0.676075468,-1.6034069282,-0
.5512391467\C,1.0398630772,-0.6526218687,-1.6824987861\C,0.579751565,0
.7689507159,-1.3292768649\C,-0.0238510927,0.3903067099,2.4767947542\C,
-0.979142735,2.2080270084,0.8465698753\C,-1.7063612669,1.0214481865,0.
9619743086\C,-1.2173689639,0.0531960101,1.8209592142\H,1.1328121565,-1
.848581795,1.5363733613\H,2.5179992785,-1.4789727639,0.5332754092\H,-0
.3986595742,-1.4873548848,-0.3351474554\H,0.5811173269,-0.9930937337,-
2.6143355113\H,-0.5172056975,0.777207754,-1.3710638236\H,0.9215988072,
1.5034362279,-2.0692755155\H,-2.5260042733,0.8093990902,0.2822424758\H
,-1.5737364384,-0.9696378572,1.8331129849\H,0.4330814128,-0.2786885107
,3.1975258088\H,-1.2306226125,2.9635749922,0.1106676747\C,-0.191655180
3,2.6842355399,1.9683986847\O,0.1884197077,1.7028618279,2.844116889\O,
0.1524177249,3.8284580985,2.1872390017\H,2.1260274196,-0.6789762038,-1
.8424538201\H,2.1295125434,0.6157836991,1.7565367569\H,1.4905543585,2.
199382875,0.1267916945\C,0.8812446926,-3.1224101762,-0.8726098096\O,0.
7197612756,-3.8810948187,0.1133742273\O,1.1643152473,-3.4057016004,-2.
0573094417\Version=ES64L-G09RevE.01\State=1-A\HF=-765.7224917\RMSE=9.
282e-09\RMSEF=5.300e-06\Dipole=-1.0932558,3.7636344,1.2683836\Quadrupol
e=28.1400751,-38.4695058,10.3294306,7.5701531,6.0008597,-28.6356183\PG
=C01 [X(C12H13O4)]\@

5b(i) [product]

1\1\GINC-R3435\FTS\RM062X\6-31+G(d,p)\C12H14O4\ROOT\07-Aug-2017\0\#M0
62X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,n
oeigentest,maxcyc=200) maxdisk=2147483648\|a3\0,1\C,1.3203744722,0.25
32268302,1.192871121\C,1.1082223129,1.2276020173,0.2068771508\C,1.4622
078288,-1.2177599619,0.8410479084\C,0.8923536252,-1.5520468587,-0.5338
626124\C,1.417249567,-0.5510655544,-1.5751403112\C,0.8705999204,0.8397
85117,-1.2435357994\C,-0.3267069176,0.3437490776,2.4561316083\C,-0.962
7750582,2.1656039168,0.6850794532\C,-1.7266144559,0.9963669,0.68022823
5\C,-1.3943826886,0.023489261,1.6071862182\H,1.0082961413,-1.860258678
8,1.6040435731\H,2.5289133147,-1.4742050931,0.836518732\H,-0.204665917
1,-1.4821277054,-0.5261964003\H,1.1069285327,-0.847385832,-2.580969863
9\H,-0.200682132,0.8354650007,-1.4766223732\H,1.3265426624,1.593184032
5,-1.8933459351\H,-2.4404162532,0.8045146448,-0.1149287968\H,-1.791095
6836,-0.9845322272,1.5835595215\H,0.009211552,-0.3355405654,3.23255807
45\H,-1.0905748719,2.9325031741,-0.0712086853\C,-0.3832567638,2.640077
3752,1.9369180396\O,-0.1463814318,1.6454118472,2.8517467378\O,-0.08230
24061,3.7764724701,0.25114032163\H,2.5142441025,-0.5513644984,-1.547178
3766\H,1.9288356017,0.52177892006,2.0369389834\H,1.5327407718,2.2122098
303,0.3807237704\C,1.2372860721,-2.9693140707,-0.9269397938\O,2.007176
8064,-3.6981809591,-0.3499906398\O,0.582261332,-3.3527783673,-2.042976
0712\H,0.8645739639,-4.2573883228,-2.2485156844\Version=ES64L-G09RevE
.01\State=1-A\HF=-766.2678248\RMSE=8.231e-09\RMSEF=1.055e-06\Dipole=-0.
4015979,-1.452658,-1.4003517\Quadrupole=4.9817415,-10.0238741,5.042132
6,5.2434337,0.7045608,-7.3168423\PG=C01 [X(C12H14O4)]\@

5b(iii) [product]

1\1\GINC-R3502\FTS\RM062X\6-31+G(d,p)\C13H19N1O2\ROOT\07-Aug-2017\0\#
M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc
,noeigentest,maxcyc=200) maxdisk=2147483648\|a5\0,1\C,1.51964612,0.30
88930015,0.8950640409\C,1.0392310235,1.2419252752,-0.035689723\C,1.750
6277204,-1.1450036912,0.5105999063\C,0.9750131433,-1.5544099429,-0.751
2020749\C,1.2415835858,-0.5204238613,-1.8433262397\C,0.6126667709,0.81
42560926,-1.4315909809\C,0.1155753016,0.2393490179,2.4212309511\C,-1.0
157854916,1.9494404222,0.7925436919\C,-1.6320708198,0.70228623,0.91523
66922\C,-1.0403036897,-0.2113972175,1.770228683\H,1.5069607249,-1.8113
787072,1.3473308004\H,2.8252474925,-1.2721314724,0.3185001505\H,-0.099
962288,-1.5048762036,-0.5214566468\H,0.8173908096,-0.8706704065,-2.789
9295207\H,-0.4764448835,0.7038836783,-1.4904359189\H,0.8823466524,1.60
2951253,-2.1410679373\H,-2.442154261,0.4175196864,0.2509950284\H,-1.31
6449382,-1.258588075,1.8082479118\H,0.6534768877,-0.3850500009,3.12689
24698\H,-1.3551604533,2.6840309282,0.0704027181\C,-0.2888714698,2.5061
672589,1.9278201314\O,0.2123105643,1.5597887705,2.7852042288\O,-0.0768
264739,3.6737980374,2.1512220631\H,2.3215202178,-0.3880504515,-1.98658
15454\H,2.2234342974,0.702862802,1.6261722474\H,1.3729216449,2.2700013

899,0.074514418\N,1.207962554,-2.9246687898,-1.2108476182\C,2.57677485
95,-3.224651363,-1.5956100187\H,2.5995313287,-4.2070925715,-2.07643119
52\H,2.9397049048,-2.4923887732,-2.320225766\H,3.2790326398,-3.2538524
048,-0.7431201441\C,0.6996725381,-3.9245581796,-0.289354425\H,1.292029
457,-4.0130458441,0.6395436284\H,-0.3335862295,-3.685541468,-0.0184677
312\H,0.7039992033,-4.9030244199,-0.7791792757\Version=ES64L-G09RevE.
01\State=1-A\HF=-711.6560536\RMSE=3.407e-09\RMSF=9.926e-06\Dipole=0.16
36509,-1.8876558,-0.8962351\Quadrupole=7.9822472,-8.3771874,0.3949402,
0.5765057,1.1749652,-11.8422066\PG=C01 [X(C13H19N1O2)]\@

5b(iv) [product]

1\1\GINC-R1515\FTS\RM062X\6-31+G(d,p)\C13H20N1O2(1+)\ROOT\07-Aug-2017\
0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,ca
lcf, noigentest, maxcyc=200) maxdisk=2147483648\la5\1,1\C,1.208583423
9,-0.0616981681,0.8292522416\C,0.7988473562,0.5200478692,-0.3894951135
\C,0.8050689531,-1.4867813961,1.1776048038\C,0.6220295245,-2.339471790
6,-0.079126398\C,-0.4306065743,-1.6571208429,-0.9542192825\C,0.0531074
36,-0.2880937021,-1.4487235289\C,0.3024771701,1.1740942757,2.354136667
5\C,-0.6671970716,2.0543685723,0.0869565721\C,-1.557480619,1.361721770
1,0.9205932204\C,-1.0469251863,0.8936781965,2.1172597058\H,-0.17017000
62,-1.5128468105,1.6746855742\H,1.5084030472,-1.9309352915,1.886356261
6\H,0.3391024972,-3.367695958,0.169519829\H,-1.3132275672,-1.531532660
8,-0.3184391267\H,-0.7967818674,0.2602171259,-1.8612655546\H,0.7335632
463,-0.4199340675,-2.3050724509\H,-2.5541279024,1.1009784543,0.5778642
188\H,-1.5886824975,0.2219368428,2.7723436573\H,0.8123307802,0.8401857
06,3.2518851194\H,-0.9759432646,2.4183965476,-0.887662465\C,0.40156656
99,2.8526210273,0.7042694373\O,0.8590210704,2.331303956,1.8892014031\O
,0.92369201,3.8296451606,0.241832704\H,-0.7491626602,-2.282694775,-1.7
919506655\H,2.1560539907,0.2828857235,1.234863965\H,1.4541734445,1.282
0550393,-0.8061999734\N,1.9449466313,-2.4681158328,-0.8336843892\C,3.0
323442927,-3.0590341283,0.0076773418\H,3.9092132865,-3.2204150774,-0.6
183581153\H,3.2816283698,-2.3740893761,0.8149034567\H,2.6790385615,-4.
0102363558,0.4090653069\C,1.8062956428,-3.2346997002,-2.109977334\H,1.
4403764355,-4.2343914279,-1.8699715518\H,1.1081750749,-2.7266894724,-2
.7713041418\H,2.7834848491,-3.3002614926,-2.5873038405\H,2.2281055527,
-1.5056139406,-1.0610475548\Version=ES64L-G09RevE.01\State=1-A\HF=-71
2.0330856\RMSE=6.450e-09\RMSF=7.281e-06\Dipole=0.8027871,-5.264428,-1.
3005859\Quadrupole=2.0581156,-3.3086088,1.2504931,-14.9532167,-3.99102
14,7.2847739\PG=C01 [X(C13H20N1O2)]\@

5d(ii) [product]

1\1\GINC-R1249\FTS\RM062X\6-31+G(d,p)\C12H13O4(1-)\ROOT\07-Aug-2017\
0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calc
fc, noigentest, maxcyc=200) maxdisk=2147483648\la6\1,1\C,0.8704916956
,0.3588705946,1.402810765\C,0.7080482515,1.2277656677,0.3109776272\C,0.
.6130277749,-1.1377287962,1.2683050394\C,0.6455699931,-1.6645753289,-0
.1718197108\C,-0.0979958822,-0.7092242325,-1.1041292132\C,0.5592799344
,0.676912959,-1.0898362646\H,-0.38733355,-1.3112894954,1.6942598759\H,
1.3217475812,-1.726983441,1.8594425801\H,0.1294360361,-2.6344811817,-0
.165756811\H,-1.1510198529,-0.6321914825,-0.7913616478\H,-0.0042854041
,1.3916308803,-1.7017147968\H,1.5379686112,0.5336606055,-1.5592555994\
C,2.8213831667,0.5457692943,1.9930523015\C,2.7930768797,2.2956066124,0
.0484625182\C,3.5510970796,1.1374590169,-0.1579630942\C,3.5780605999,0
.2052265891,0.862416\H,2.7894509557,-0.0962635408,2.8669965466\H,2.623
4639447,3.0169890714,-0.7435401022\H,3.9362145106,0.8858075782,-1.1407
639111\H,3.9132680804,-0.8167212173,0.7185269394\C,2.6184808893,2.8132
601518,1.3921151167\O,2.7455978054,1.8736745197,2.3761806006\O,2.36162
42167,3.960609329,1.7091335853\H,-0.0697823351,-1.1008553771,-2.125286
6528\H,0.5655975008,0.774829582,2.3633879386\H,0.3107152343,2.21998473
23,0.5101354967\C,2.1057654492,-2.0082983823,-0.6309036749\O,2.7640283
736,-2.6893504619,0.1940071118\O,2.4690684597,-1.5855412466,-1.7526295
645\Version=ES64L-G09RevE.01\State=1-A\HF=-765.7314646\RMSE=7.291e-09
\RMSF=5.839e-06\Dipole=-1.4406971,1.2309799,0.699824\Quadrupole=13.348
552,-20.4112216,7.0626696,4.4489713,0.7388629,-16.4234265\PG=C01 [X(C1
2H13O4)]\@

5d(i) [product]

1\1\GINC-R1248\FTS\RM062X\6-31+G(d,p)\C12H14O4\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc, noeigentest,maxcyc=200) maxdisk=2147483648\|a4\|0,1\C,1.1646533174,0.2300722499,1.4956417087\C,0.7393592761,1.1675111091,0.5425495669\C,1.2884617911,-1.2535611888,1.1680575357\C,0.604105575,-1.6356171049,-0.1454524475\C,0.9578773643,-0.6163466339,-1.2419013539\C,0.3800131988,0.7465775872,-0.868807209\H,0.8584675597,-1.8367863351,1.9892187394\H,2.3349473634,-1.565040068,1.0901706401\H,-0.4870498987,-1.6440320852,-0.030732685\H,0.5605286858,-0.9404088167,-2.2084417808\H,-0.7168395789,0.6887206778,-0.92345578\H,0.6793773578,1.5009152899,-1.6022073898\C,3.1191986853,0.8370640092,2.0328622327\C,2.5214678164,2.4960201446,0.1026126379\C,3.4987147948,1.5361161467,-0.1794703954\C,3.823635709,0.6566755018,0.8379968576\H,3.2808608634,0.2012110551,2.8966820394\H,2.1540588891,3.1742729672,-0.6597163535\H,3.866658,1.4014355742,-1.1919715598\H,4.4227917613,-0.2322119473,0.68308615\C,2.4030795164,3.0066759564,1.4674403398\O,2.7707408482,2.1048368394,2.4295305619\O,1.9907684495,4.0918970758,1.798764662\H,2.0501985386,-0.5594048022,-1.3308665783\H,0.8875574703,0.4571699887,2.5218380379\H,0.2102960037,2.0436454403,0.9102613162\C,1.0231879654,-3.0168282364,-0.5910648533\O,2.0274320849,-3.5969665504,-0.2540702151\O,0.1491659762,-3.545367987,-1.4718697341\H,0.4979376158,-4.4078658576,-1.7457406906\|Version=ES64L-G09RevE.01\|State=1-A\|HF=-766.2672511\|RMSD=5.686e-09\|RMSF=2.706e-06\|Dipole=-0.4089403,-1.5550552,-1.1921446\|Quadrupole=5.3772008,-11.7605906,6.3833898,1.6877209,-0.4970633,-6.8623005\|PG=C01 [X(C12H14O4)]\|@

5d(iii) [product]

1\1\GINC-R1234\FTS\RM062X\6-31+G(d,p)\C13H19N1O2\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc, noeigentest,maxcyc=200) maxdisk=2147483648\|a3\|0,1\C,0.9848732144,0.2039740036,1.1309286365\C,0.9511605108,1.1135376469,0.0740296996\C,1.2113821186,-1.2475936576,0.7651075569\C,0.2316879192,-1.6546517186,-0.3536105065\C,0.3676676669,-0.6903077552,-1.5629090439\C,1.2678031775,0.5303007766,-1.2756861785\H,1.0747808427,-1.8712679895,1.6517957831\H,2.2339729747,-1.4106473569,0.399521978\H,-0.789859103,-1.5584107648,0.0700801773\H,-0.6210165303,-0.3443688466,-1.881083235\H,1.1713172823,1.2730557808,-2.072184391\H,2.3120686401,0.1909382842,-1.2762321506\C,2.6510813001,0.7803563106,2.3222813724\C,2.7914458749,2.5115917034,0.3453012894\C,3.7895753016,1.5397027076,0.4043026801\C,3.7205757521,0.6190358274,1.4391940643\H,2.5039672686,0.1262057443,3.1748467233\H,2.7252133644,3.2118810862,-0.4798792693\H,4.4971299497,1.4246808108,-0.4107193467\H,4.3315178729,-0.2743579847,1.4784509594\C,2.1509652316,2.9611687183,1.5772500823\O,2.1755565728,2.0378541258,2.5927112082\O,1.6025610678,4.0212027437,1.7616987908\H,0.8060331434,-1.2464709426,-2.3973718311\H,0.3539101872,0.4062931437,1.9931404528\H,0.3291333419,2.0017939631,0.1393316254\N,0.4339516069,-3.0402422981,-0.7965113579\C,0.4939269998,-3.988381086,0.3069874307\H,0.5303063817,-5.0015897293,-0.100752259\H,1.3965771831,-3.8408419335,0.9020134713\H,-0.3875791329,-3.9189738818,0.9733953574\C,-0.6346406113,-3.4402815235,-1.7041114367\H,-1.6239585566,-3.4279762545,-1.207884475\H,-0.6806386488,-2.7749789144,-2.5681454763\H,-0.4445521648,-4.4530147396,-2.0684563818\|Version=ES64L-G09RevE.01\|State=1-A\|HF=-711.6546633\|RMSD=4.507e-09\|RMSF=3.341e-06\|Dipole=0.2104493,-1.9692562,-0.8174303\|Quadrupole=6.8247313,-10.477327,3.6525957,1.7797567,0.7650495,-10.499498\|PG=C01 [X(C13H19N1O2)]\|@

5d(iv) [product]

1\1\GINC-R1241\FTS\RM062X\6-31+G(d,p)\C13H20N1O2(1+)\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc, noeigentest,maxcyc=200) maxdisk=2147483648\|a3\|1,1\C,1.0147090666,0.1865291377,1.1374796884\C,0.9948805124,1.1063724897,0.0851123085\C,1.2537302071,-1.262630227,0.7608618062\C,0.2563571588,-1.6164859775,-0.3520316989\C,0.4078782528,-0.6801740527,-1.5766532574\C,1.3116284114,0.5338956388,-1.2746036039\H,1.1186867507,-1.8974455457,1.6393569675\H,2.2799526998,-1.4055152543,0.3913458168\H,-0.7589911921,-1.5678498138,0.0564310216\H,-0.5784055991,-0.3373753996,-1.9001732783\H,1.1994632206,1.2780477026,-2.0658149251\H,2.3577092215,0.2036062529,-1.2921893201\C,2.6745284763,0.7901799035,2.3849911583\C,2.7540456829,2.4767737891,0.3651827179\C,3.7887350533,1.5412749851,0.4457120924\C,3.7409971385

,0.6384350694,1.4961129896\H,2.5446857214,0.1450143931,3.2478110123\H,
2.683658102,3.1738973227,-0.463232854\H,4.5134112815,1.4454665406,-0.3
56757404\H,4.3955169405,-0.2218926464,1.5712424235\C,2.1107010001,2.94
20275094,1.5981926708\O,2.146465626,2.0247404092,2.62435716\O,1.538769
9423,3.9855856427,1.7601173278\H,0.8429842617,-1.227653198,-2.42399383
71\H,0.3730006732,0.3640460286,1.9955513324\H,0.3442972867,1.974180775
4,0.1426760125\N,0.3926982772,-3.0691400754,-0.8153268863\C,0.48266505
31,-4.0541569151,0.3074692336\H,0.4453728988,-5.0603711597,-0.10943503
75\H,1.4161166756,-3.9117902835,0.8471744328\H,-0.3684305996,-3.894359
7459,0.9714515715\C,-0.7273010035,-3.4497451046,-1.7356118861\H,-1.651
4225978,-3.444330058,-1.1558552428\H,-0.7928800776,-2.731617663,-2.550
3647072\H,-0.5389561256,-4.4483996506,-2.1290731931\H,1.2675436027,-3.
12614682,-1.3480886125\Version=ES64L-G09RevE.01\State=1-A\HF=-712.029
2853\RMSD=6.839e-09\RMSF=1.060e-05\Dipole=-1.1222403,-6.1820274,-2.596
9747\Quadrupole=-2.8353778,7.9522795,-5.1169017,13.3890921,5.6500757,2
.0117015\PG=C01 [X(C13H20N1O2)]\@

3c(ii)[product]

1\1\GINC-R696\FTS\IRM062X\6-31+G(d,p)\C11H11O4(1-)\ROOT\07-Aug-2017\0\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcf c,noeigentest,maxcyc=200) maxdisk=1610612736\|a1\|-1,1\C,1.0240409252, 0.9389134597,0.7416750891\C,0.5205209958,0.0339688452,1.677033206\C,1. 2498337246,0.2184518903,-0.5826087898\C,1.1776551969,-1.2894893408,-0. 2407358181\C,0.425923156,-1.3546409404,1.0992223867\H,2.1860014925,0.4 810486331,-1.0854550036\H,0.4369059606,0.4867983261,-1.270450464\H,2.1 937250083,-1.6801844479,-0.1304535298\H,0.7971228711,-2.1417951284,1.7 645891111\H,-0.6261364968,-1.5891011344,0.8761186462\C,2.9737796995,1. 3714281874,1.36254185\C,2.2314906639,-0.0710162732,3.4362972066\C,2.35 24574571,1.3022649539,3.6318175274\C,2.7643146177,2.0738299672,2.55573 55342\H,3.2977898033,1.8629352883,0.4515324358\H,1.8253325893,-0.72918 72324,4.195556805\H,1.9970439356,1.7585727415,4.5513790814\H,2.7058681 051,3.155673747,2.5468695326\C,3.0484428666,-0.7284970116,2.4296491375 \O,3.4742225616,0.0974894257,1.4158316565\O,3.3893886348,-1.8897735865 ,2.4201440234\H,0.7148557226,1.9808495389,0.7586392046\H,-0.0812783929 ,0.346175459,2.5245129109\C,0.4889255743,-2.0609525146,-1.4146748661\O ,1.1320002718,-2.0298907545,-2.4890139822\O,-0.6274869444,-2.576612098 3,-1.1720128913\Version=ES64L-G09RevE.01\State=1-A\HF=-726.4154844\RM SD=8.277e-09\RMSF=2.040e-06\Dipole=1.0949683,4.4860076,4.3156318\Quadr upole=3.3894842,6.6794201,-10.0689043,-7.2862053,-15.8877254,-16.29797 73\PG=C01 [X(C11H11O4)]\@

3c(i) [product]

1\1\GINC-R2463\FTS\IRM062X\6-31+G(d,p)\C11H12O4\ROOT\07-Aug-2017\0\#M0 62X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcf,c,n oeigentest,maxcyc=200) maxdisk=1610612736\|a1\|0,1\C,1.3733074898,0.98 84933694,0.5345191698\C,0.4882225251,0.4776198594,1.4865812006\C,1.523 0995317,-0.0072013953,-0.6080784368\C,0.9496124813,-1.3275219829,-0.02 72489706\C,-0.0148093764,-0.8925353585,1.0866373433\H,2.5474039514,-0. 1372922144,-0.9687340305\H,0.9186905711,0.3363333809,-1.4579703401\H,1 .7695367444,-1.9229707572,0.3859349544\H,-0.0535111552,-1.6180942363,1 .9042089229\H,-1.0303051445,-0.7974187232,0.6809116516\C,3.2822523176, 0.9206975755,1.4373239822\C,1.7650057933,0.1303092403,3.4358569948\C,2 .3279452691,1.4039950412,3.5352797617\C,3.1295713536,1.8279391722,2.49 03487005\H,3.8928918052,1.140964863,0.5682059418\H,1.0525923069,-0.240 217332,4.1643230654\H,2.0213401141,2.0804434294,4.3266246555\H,3.45815 37947,2.8536881674,2.3748147597\C,2.4572343444,-0.9028586379,2.6814520 949\O,3.2953488288,-0.4236975434,1.7022101181\O,2.3417355602,-2.099665 9495,2.8128540521\H,1.4207179331,2.0514509199,0.3249860474\H,-0.108955 3836,1.1152461514,2.1268520023\C,0.28766354,-2.1530101813,-1.099258561 2\O,-0.8935396142,-2.3815274305,-1.201571071\O,1.1871410443,-2.6071989 5,-1.9966442817\H,0.6992133736,-3.1143504772,-2.6635997272\Version=ES 64L-G09RevE.01\State=1-A\HF=-726.9719169\RMSD=4.288e-09\RMSF=3.238e-06 \Dipole=0.1456378,2.0590385,-0.2865236\Quadrupole=-6.1994926,1.8401231 ,4.3593695,1.7771859,-5.2848967,6.4515136\PG=C01 [X(C11H12O4)]\@

3c(iii) [product]

1\1\GINC-R537\FTS\IRM062X\6-31+G(d,p)\C12H17N1O2\ROOT\07-Aug-2017\0\#M

062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc, noeigentest,maxcyc=200) maxdisk=1610612736\|a1\|0,1\C,1.2793797886,0.9 295793996,0.4852198677\C,0.4582445791,0.2991555512,1.4216050409\C,1.54 9653836,-0.0250462501,-0.6679517901\C,1.1619712573,-1.4177487291,-0.12 74344674\C,0.1452902053,-1.1170757734,0.9944730267\H,2.5799663886,0.01 0598723,-1.0379648603\H,0.8832782559,0.2293431019,-1.5036586375\H,2.05 29501151,-1.8964563679,0.3163725183\H,0.1818309299,-1.846767086,1.8093 923641\H,-0.867831447,-1.1328688243,0.5663201617\C,3.1748261982,1.0830 219074,1.4161161856\C,1.7387300821,0.1098275552,3.3925922922\C,2.13780 82705,1.4432356156,3.4993438197\C,2.8966300602,1.9639125496,2.46586541 02\H,3.7630551712,1.3769820988,0.5533958305\H,1.0673070785,-0.34645610 18,4.1112626598\H,1.7372792914,2.0761241143,4.2847836385\H,3.095708603 6,3.0227863658,2.353240084\C,2.5685325289,-0.8292507971,2.6534687464\O ,3.3509767247,-0.2491557663,1.6832050747\O,2.6096373119,-2.0296398668, 2.7959512666\H,1.203215062,1.9946922633,0.2960001591\H,-0.22497646,0.8 444771012,2.061332196\N,0.6031858626,-2.2846083449,-1.1651358688\C,1.5 715659257,-2.5023825383,-2.2309793606\H,1.1377000085,-3.1656430113,-2. 9839576816\H,1.8213511438,-1.5577702573,-2.7197332245\H,2.5068708569,- 2.9618491435,-1.8592234345\C,0.208040923,-3.5694364567,-0.6009182538\H ,1.054934876,-4.0922605714,-0.1194645699\H,-0.5789694428,-3.4331064482 ,0.1439798902\H,-0.1876639859,-4.2064140124,-1.396418084\|Version=ES64 L-G09RevE.01\State=1-A\HF=-672.3621357\|RMSD=6.656e-09\|RMSF=1.819e-05\|D ipole=-0.5053584,1.6132652,-0.2902885\|Quadrupole=-3.182924,3.2105528,- 0.0276288,3.8474342,-5.9619672,5.5432517\|PG=C01 [X(C12H17N1O2)]\|@

3c(iv) [product]

1\1\GINC-R3114\FTS\RM062X\6-31+G(d,p)\C12H18N1O2(1+)\|ROOT\07-Aug-2017\ 0\|#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,ca lcfc,noeigentest,maxcyc=200) maxdisk=1610612736\|a1\|1,1\C,1.266867133 8,0.9793723339,0.4799346622\C,0.4382788425,0.3503469669,1.4177533355\C ,1.5019276499,0.0346324209,-0.6944411267\C,1.1335308631,-1.3390602682, -0.1121073316\C,0.0747502257,-1.0486061465,0.9640295865\H,2.5211734346 ,0.0610457816,-1.0910087054\H,0.8163029194,0.3073508681,-1.5121199104\ H,2.0055681429,-1.8266969218,0.3307709432\H,0.0747525513,-1.7947750967 ,1.7633600013\H,-0.9333356923,-1.020370739,0.5182481655\C,3.1651661155 ,1.0647080437,1.3818150177\C,1.7198588105,0.0473629104,3.3344795417\C, 2.1683333325,1.3633340136,3.497466561\C,2.9217805531,1.9044085593,2.47 54793577\H,3.7731992003,1.3805874739,0.5404446278\H,1.0463820627,-0.41 74665865,4.0464455288\H,1.8117891446,1.9675748038,4.3248415028\H,3.168 958799,2.9575046641,2.4154840644\C,2.49522878,-0.8817529198,2.5313383 388\O,3.2956725043,-0.2867088179,1.5871086576\O,2.4444945858,-2.092814 9362,2.5608408612\H,1.1980738029,2.0427742361,0.2852039845\H,-0.241157 6197,0.8949262185,2.0601771381\N,0.6421236644,-2.3192471871,-1.1502899 941\C,1.6604890318,-2.5430533498,-2.2230662085\H,1.2670710549,-3.26405 50648,-2.9392122808\H,1.8731167423,-1.5980529234,-2.7201080915\H,2.563 7749294,-2.9337107315,-1.7520545312\C,0.2489660367,-3.6190280738,-0.51 5925113\H,1.1087519625,-3.9925200614,0.0430704378\H,-0.5872029515,-3.4 491643553,0.159892605\H,-0.0354546698,-4.3219201995,-1.2985130931\H,-0 .1933917237,-1.9160349155,-1.5889785328\|Version=ES64L-G09RevE.01\Stat e=1-A\HF=-672.7475363\|RMSD=5.630e-09\|RMSF=2.971e-06\|Dipole=-1.845914,- 0.4617503,-2.9857762\|Quadrupole=-9.7914957,3.6065559,6.1849398,9.82347 1,1.9775232,18.1402805\|PG=C01 [X(C12H18N1O2)]\|@

5e(ii) [product]

1\1\GINC-R1494\FTS\RM062X\6-31+G(d,p)\C12H13O4(1-)\|ROOT\07-Aug-2017\0 \|#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calc fc,noeigentest,maxcyc=200) maxdisk=2147483648\|a6\|-1,1\C,1.59214852,0 .7454930916,0.3777889344\C,0.7451824409,-0.0633808397,1.1412133298\C,2 .4179042986,0.1475715265,-0.7587811085\C,1.8100767885,-1.1635581442,-1 .2547861599\C,1.6479462787,-2.1118636264,-0.0646103628\C,0.6057562217, -1.5490080319,0.9048352983\H,3.4499884591,-0.0444412523,-0.4330059117\ H,2.4351272972,0.8749068658,-1.574149162\H,2.4935964928,-1.6217716329, -1.982586005\H,2.6081361186,-2.24529413,0.4520853915\H,0.6033264589,-2 .1093588165,1.8475608483\H,-0.3839186517,-1.6845037858,0.444332786\C,3 .1134353285,1.3175353771,1.6943478249\C,1.6138829605,0.0278682511,3.42 38996293\C,1.6610849535,1.4154365433,3.5423889218\C,2.4629859005,2.108 2385491,2.6501663135\H,3.771159443,1.7450656309,0.94535772\H,0.9301735

624,-0.5777721247,4.0075810576\H,0.9766438677,1.9323106266,4.208812495
6\H,2.4175161609,3.1834730465,2.5256798118\C,2.7521018197,-0.687741077
6,2.8756986618\O,3.5557390059,0.0672797124,2.0565765973\O,3.0537456868
,-1.8434405448,3.0879670848\H,1.3036655664,-3.086855532,-0.4181565311\
H,1.2470500197,1.762490283,0.2207740918\H,-0.1007343487,0.4196697854,1
.6217794374\C,0.4424549972,-0.9461951566,-1.994736276\O,-0.2070831318,
-1.9950836039,-2.2156521908\O,0.1486804845,0.23879101,-2.2838435278\W
ersion=ES64L-G09RevE.01\State=1-A\HF=-765.719373\RMSD=4.822e-09\RMSF=2
.193e-06\Dipole=1.7469441,2.2714018,3.7827599\Quadrupole=4.6063696,11.
9649955,-16.5713651,-0.7613681,-26.8562675,-1.0271936\PG=C01 [X(C12H13
O4)]\@

5e(i) [product]

1\1\GINC-R1489\FTS\RM062X\6-31+G(d,p)\C12H14O4\ROOT\07-Aug-2017\0\#M0
62X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,n
oeigentest,maxcyc=200) maxdisk=2147483648\|a2\|0,1\C,1.4970299278,0.71
91436858,0.434773238\C,0.8021392484,-0.2668101343,1.1509603373\C,2.435
8374516,0.3383902631,-0.709102415\C,2.1401737387,-1.0534787514,-1.2670
544313\C,2.0868755113,-2.0670632387,-0.1141737055\C,0.9259007013,-1.74
36143426,0.8278971434\H,3.4804974504,0.3265181511,-0.3785074673\H,2.34
46680432,1.0905176277,-1.4973833599\H,2.9312568029,-1.3518057438,-1.96
62109933\H,3.0363825503,-2.0193045359,0.4293034717\H,1.0124005764,-2.3
519004971,1.7340567526\H,-0.0206241605,-2.0397054682,0.3507609452\C,2.
911109685,1.4786272944,1.7975277879\C,1.5902205019,-0.1832287705,3.333
0270376\C,1.4167844589,1.1794179019,3.5898674262\C,2.1112708127,2.0630
903588,2.7861767915\H,3.505391889,2.0754737995,1.1136221557\H,1.009209
7837,-0.9392776083,3.8494521441\H,0.6518387633,1.516860915,4.281727710
6\H,1.9095459358,3.1271565607,2.7619030362\C,2.8565700297,-0.654639825
6,2.7907315113\O,3.5390545314,0.2855201794,2.0588612506\O,3.3255042571
,-1.7641565966,2.9055241122\H,1.9760668556,-3.084085004,-0.4985488784\
H,0.9823690894,1.6655553491,0.310309361\H,-0.1433461316,0.0260583027,1
.5956139432\C,0.8510350259,-1.0588199647,-2.0617230937\O,0.1479941486,
-0.1022457299,-2.284863544\O,0.5489602381,-2.2907659575,-2.5245422\H,-
0.2739847162,-2.2140052202,-3.031453068\|Version=ES64L-G09RevE.01\Stat
e=1-A\HF=-766.2704695\RMSD=8.088e-09\RMSF=4.632e-06\Dipole=-0.9530676,
0.8618081,-0.3647931\Quadrupole=-2.0956317,2.3613432,-0.2657114,6.2879
181,-7.8783779,8.0493523\PG=C01 [X(C12H14O4)]\@

5e(iii) [product]

1\1\GINC-R1243\FTS\RM062X\6-31+G(d,p)\C13H19N1O2\ROOT\07-Aug-2017\0\#
M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc
,noeigentest,maxcyc=200) maxdisk=2147483648\|a3\|0,1\C,1.2908638634,0.
9198852587,0.3891296822\C,0.5122396356,0.2768465655,1.3673307741\C,1.6
403349886,0.1989933916,-0.9074390397\C,1.4024978204,-1.3121674056,-0.8
432164859\C,-0.000521704,-1.575846346,-0.2825645291\C,-0.0561834138,-1
.1224543805,1.1789488148\H,2.6788748657,0.3694018903,-1.210228851\H,1.
014253621,0.6311357925,-1.6995660624\H,2.1290246745,-1.7360595991,-0.1
377038267\H,-0.2531300504,-2.6401189093,-0.3475091117\H,0.4787689233,-
1.8601000872,1.7883439803\H,-1.0908389359,-1.1162971821,1.5387221563\C
,3.1829399354,1.1405012171,1.2339146575\C,1.9213759177,-0.0454722969,3
.1976905915\C,2.291089645,1.287847725,3.406779036\C,2.9538800516,1.922
3685872,2.375981156\H,3.7130427252,1.533533577,0.3732855342\H,1.308997
5981,-0.5868976919,3.9103098168\H,1.9278637471,1.8309272604,4.27343372
98\H,3.1146409596,2.9932036438,2.342814437\C,2.7341945604,-0.885676803
8,2.3316891885\O,3.4492816565,-0.1980422095,1.3856710008\O,2.802913949
9,-2.0949594333,2.3524691087\H,-0.7436228752,-1.0242695759,-0.87454080
26\H,1.1489444552,1.9928220157,0.293859361\H,-0.0416730107,0.918104666
,2.0447825335\N,1.6989937494,-1.9308038006,-2.139159994\C,2.0364651372
,-3.339562281,-2.0140009471\H,2.3799934215,-3.7147180753,-2.9828691878
\H,2.8454278721,-3.4638864539,-1.2900014003\H,1.1827953726,-3.96550245
38,-1.6945907007\C,0.6678888464,-1.7466142493,-3.1470706841\H,-0.25269
95708,-2.320700269,-2.936587046\H,0.3991865917,-0.6912543093,-3.240216
5999\H,1.0541479757,-2.0772437774,-4.1157842896\|Version=ES64L-G09RevE
.01\State=1-A\HF=-711.6568087\RMSD=8.309e-09\RMSF=4.513e-06\Dipole=-1.
0173635,1.5914173,-0.0513972\Quadrupole=-2.9527307,2.2166914,0.7360393
,3.7482377,-2.6467526,5.8531221\PG=C01 [X(C13H19N1O2)]\@

5e(iv) [product]

1\1\GINC-R104\FTS\RM062X\6-31+G(d,p)\C13H20N1O2(1+)\ROOT\07-Aug-2017\0
\\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,cal
cfc, noeigentest, maxcyc=200) maxdisk=2147483648\|a3\|1,1\C,1.2781977983
,0.9780297527,0.3897759994\C,0.5048913712,0.3152824504,1.3629322301\C,
1.605758541,0.2651651228,-0.921632552\C,1.3894911065,-1.2396660969,-0.
7890091934\C,-0.0273728368,-1.5272878139,-0.3185008881\C,-0.131437736,
-1.049708146,1.1382930115\H,2.6411154212,0.4672221169,-1.2272607542\H,
0.9511327958,0.6740212109,-1.7024066731\H,2.1018199384,-1.6572420838,-
0.0724173264\H,-0.2722169502,-2.5933140117,-0.3618898085\H,0.313894728
8,-1.8148282991,1.7826690402\H,-1.1866823229,-0.9812868557,1.416820574
9\C,3.177644855,1.1722477299,1.2063694311\C,1.9501994666,-0.1594672998
,3.1014111014\C,2.3445334919,1.1511935681,3.4080791087\C,2.9777021393,
1.8617718847,2.4128712325\H,3.7082833543,1.6323680085,0.3788811073\H,1
.3524123995,-0.7479608832,3.7890262218\H,2.0225983792,1.6204410684,4.3
317210415\H,3.1600294793,2.9282346036,2.4665489314\C,2.7119701339,-0.9
318223328,2.1376702071\O,3.4344758167,-0.1794576471,1.2467876163\O,2.7
112907295,-2.1385339708,1.9987995591\H,-0.7464815257,-0.9853926294,-0.
9447448542\H,1.1329372884,2.0484740575,0.2889138567\H,-0.0154452185,0.
9483032656,2.072722451\H,1.7460675227,-1.9482096969,-2.0928421378\C,2.0
834827668,-3.3887211696,-1.8544450143\H,2.4135591749,-3.8328991314,-2.
7935710519\H,2.8699317031,-3.4447044773,-1.1016099437\H,1.1898818675,-
3.8986498388,-1.4958567738\C,0.7270333769,-1.808120359,-3.1767450668\H
, -0.1642504135,-2.3637343687,-2.8870342614\H,0.4857143462,-0.755479596
, -3.3173849394\H,1.1387463625,-2.2225837012,-4.0969311428\H,2.60511664
84,-1.4957984312,-2.4222863392\|Version=ES64L-G09RevE.01\State=1-A\HF=
-712.0446279\RMSD=2.694e-09\RMSF=4.449e-06\Dipole=-0.9803148,-0.110150
4,-3.3007008\Quadrupole=-12.9741625,-1.6142929,14.5884555,4.623545,-1.
8250771,18.1425568\PG=C01 [X(C13H20N1O2)]\@

3d(ii) [product]

1\1\GINC-R1209\FTS\RM062X\6-31+G(d,p)\C11H11O4(1-)\ROOT\07-Aug-2017\0\#M0
62X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calc
fc, noeigentest, maxcyc=200) maxdisk=1610612736\|a6\|1,1\C,1.6181693079
,0.7942258147,0.8459049083\C,0.7989432103,0.0737788194,1.722178693\C,1
.7539765865,0.0048489511,-0.4561358009\C,1.3543350895,-1.4241495567,-0
.0468480167\C,0.286360956,-1.1791800326,1.0406404469\C,0.492766705,2.4
630246117,0.2896050942\C,-1.0760604158,1.6120497354,2.230513079\C,-0.3
058896959,2.7450259915,2.4880930875\C,0.5012348913,3.2221019958,1.4679
028494\H,2.7584451427,0.0626178984,-0.8828215453\H,1.0553438948,0.3531
219716,-1.2275917799\H,2.2228146295,-1.8925925832,0.4423090491\H,0.169
3426155,-2.0202951503,1.7278604217\H,-0.6916210813,-1.0296724053,0.560
1324156\H,-0.2446812868,3.1505897822,3.4939559765\H,1.2657622764,3.974
329372,1.6223004451\H,1.0822492213,2.7334669871,-0.5801342447\H,-1.669
0407376,1.1305815125,2.9991187416\C,-1.4969652514,1.3328664313,0.86911
05204\O,-0.6664617215,1.8476239638,-0.0996240588\O,-2.4843786802,0.723
2657756,0.5276038174\H,2.4398765342,1.3960199365,1.2209409297\H,0.8688
424079,0.1596993921,2.8002787642\C,0.9399838502,-2.37413184,-1.2022859
984\O,1.3868284431,-2.0684963127,-2.333092691\O,0.2460051082,-3.356618
0616,-0.8532461041\|Version=ES64L-G09RevE.01\State=1-A\HF=-726.4069807
\RMSD=6.803e-09\RMSF=3.120e-06\Dipole=1.0147771,5.0503742,4.0263271\Qu
adrupole=8.7048995,-12.9909756,4.2860761,6.6431662,3.9216639,-19.04447
56\PG=C01 [X(C11H11O4)]\@

3d(i) [product]

1\1\GINC-R1210\FTS\RM062X\6-31+G(d,p)\C11H12O4\ROOT\07-Aug-2017\0\#M0
62X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,n
oeigentest, maxcyc=200) maxdisk=1610612736\|a1\|0,1\C,1.7910967489,0.86
96146802,0.9535206035\C,1.0278319882,0.1452875991,1.8726228492\C,2.137
0409926,-0.0034437096,-0.2471700963\C,1.3189847565,-1.2994454813,-0.06
07618184\C,0.7599220924,-1.2649430566,1.3888402722\C,0.4712797515,2.28
00571317,0.1235719435\C,-1.0596071862,1.2025409391,1.966666781\C,-0.61
98116048,2.5088047104,2.1976939915\C,0.1842635232,3.0854377254,1.23208
73076\H,3.210730567,-0.2176509705,-0.2356582203\H,1.9034216831,0.45377
44843,-1.2137421542\H,1.9613711447,-2.1800361515,-0.1763208119\H,1.314
4963744,-1.9625135109,2.0267237054\H,-0.2914888213,-1.5649375149,1.427
712061\H,-0.7808482594,2.981968729,3.161053684\H,0.7303494422,4.00774

80355,1.3896546097\H,1.0848877776,2.6258653808,-0.7014231007\H,-1.6158
542415,0.6450110756,2.7118928166\C,-1.2464932127,0.7454024925,0.598161
3713\O,-0.4721248676,1.3955846118,-0.3253430155\O,-1.9752291075,-0.148
008797,0.2271970234\H,2.5019882477,1.6172509046,1.2867772228\H,1.04600
34944,0.3558480383,2.9347962743\C,0.2610231143,-1.4886717607,-1.134586
072\O,0.1953566324,-0.8774663241,-2.1714813538\O,-0.5641100313,-2.5067
644964,-0.8321139168\H,-1.2667809986,-2.5149247647,-1.4998036414\\Vers
ion=ES64L-G09RevE.01\State=1-A\HF=-726.967844\RMSE=4.753e-09\RMSF=4.84
1e-06\Dipole=1.3561263,0.6976531,1.5128019\Quadrupole=-2.3482067,4.367
6648,-2.0194581,1.3184303,-0.927901,2.3940075\PG=C01 [X(C11H12O4)]\@

3d(iii) [product]

1\1\GINC-R1218\FTS\RM062X\6-31+G(d,p)\C12H17N1O2\ROOT\07-Aug-2017\0\#
M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc
,noeigentest,maxcyc=200) maxdisk=1610612736\la5\0,1\C,1.6468914992,0.
6412738967,1.0985072474\C,0.6101048643,0.0218698254,1.809094208\C,2.04
59162517,-0.229131709,-0.0863581525\C,1.4347756252,-1.6200251595,0.256
4004201\C,0.237082062,-1.3057121016,1.1827716491\C,0.7669119475,2.3065
309403,0.1550466201\C,-1.2688036728,1.4408666781,1.5774296571\C,-0.668
6128737,2.6321900579,1.9939020586\C,0.3994452168,3.0977709348,1.249705
4513\H,3.1318186067,-0.2702906656,-0.2131019409\H,1.6170189613,0.14777
56425,-1.0228478608\H,2.176193593,-2.1517684112,0.8672637904\H,0.10782
93261,-2.0841012783,1.9404217843\H,-0.6996851248,-1.264629637,0.616380
2679\H,-0.9398750738,3.0828985797,2.9431398417\H,1.0496229644,3.897651
6451,1.5830069661\H,1.5836796631,2.5756738702,-0.5064519765\H,-2.05198
06324,0.9614359287,2.1535769028\C,-1.2491397224,1.0885272525,0.1675311
754\O,-0.2011185498,1.627035982,-0.5372936528\O,-2.0308817596,0.367520
9029,-0.411197699\H,2.3895939219,1.2419933223,1.610962773\H,0.44581177
23,0.2040291846,2.863599352\N,1.1055118817,-2.5097020969,-0.8435308415
\C,0.2439915063,-1.9323301019,-1.8671987983\H,-0.1475782618,-2.7391671
571,-2.4938669765\H,-0.6025569058,-1.4027282953,-1.4248974408\H,0.7782
006143,-1.2247700435,-2.5260296759\C,2.2861543825,-3.1005986396,-1.447
4933876\H,2.9184032181,-2.359933284,-1.9726912989\H,2.8924555516,-3.59
27952727,-0.6813175508\H,1.9808221468,-3.8551547907,-2.1785189126\\Ver
sion=ES64L-G09RevE.01\State=1-A\HF=-672.3559789\RMSE=6.775e-09\RMSF=2.
247e-06\Dipole=1.4612397,0.7903344,1.1556071\Quadrupole=-4.1972904,1.5
976981,2.5995923,0.9393017,-4.6816297,3.7426741\PG=C01 [X(C12H17N1O2)]
\@

3d(iv) [product]

1\1\GINC-R1251\FTS\RM062X\6-31+G(d,p)\C12H18N1O2(1+)\ROOT\07-Aug-2017\
0\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,ca
lcfc,noeigentest,maxcyc=200) maxdisk=1610612736\la1\1,1\C,1.806947624
8,0.8166928059,1.0749338486\C,0.9714879887,0.1557324954,1.9813267988\C
,2.4209721812,-0.2063088139,0.1236309202\C,1.6799182796,-1.5413217721,
0.3793660281\C,0.9353839174,-1.3348249556,1.7241908975\C,0.6062820104,
1.9211231689,-0.1324219004\C,-1.2603149019,1.0524647197,1.5318405868\C
,-0.9329543411,2.4131259829,1.5916481073\C,0.0316284775,2.8762354791,0
.7230870864\H,3.4723804607,-0.3494110401,0.3918475404\H,2.4159012035,0
.1064365856,-0.9227343434\H,2.4017456701,-2.3598702014,0.4445915988\H,
1.4848459389,-1.8386066011,2.5277842169\H,-0.0761351655,-1.7560314506,
1.7250317659\H,-1.3419356097,3.0407793133,2.3759789898\H,0.4614802218,
3.8683790874,0.7909758355\H,1.3172873463,2.2065322564,-0.9008979819\H,
-1.9267610156,0.5847103643,2.2474523463\C,-1.0509394827,0.325637304,0.
3143019086\O,-0.1821822544,0.8801433481,-0.5768658058\O,-1.5260440394,
-0.7703625789,0.0151472663\H,2.4197561689,1.6510964815,1.396869842\H,0
.7591581888,0.5348572894,2.9727830958\N,0.7211500798,-1.9997380402,-0.
7084890092\C,1.210812523,-1.7850177877,-2.0977248896\H,0.5616444048,-2
.3369293962,-2.7773210936\H,1.1592616833,-0.7258934907,-2.3409218299\H
,2.2349457829,-2.1551585765,-2.1812726429\C,0.3796188899,-3.4388786801
,-0.5041386805\H,1.2572971428,-4.0467279673,-0.7327368115\H,0.07267197
02,-3.595724895,0.5290594534\H,-0.4440157886,-3.6983044559,-1.16911361
46\H,-0.1942855565,-1.4821859784,-0.5928295303\\Version=ES64L-G09RevE.
01\State=1-A\HF=-672.7604655\RMSE=7.117e-09\RMSF=4.537e-06\Dipole=1.55
74097,-0.74182,-0.0694899\Quadrupole=-9.7701046,11.4115517,-1.6414471,
-3.5284708,-5.1635598,8.2177624\PG=C01 [X(C12H18N1O2)]\@

5g(ii) [product]

1\1\GINC-R1276\FTS\IRM062X\6-31+G(d,p)\C12H13O4(1-)\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc, noeigentest,maxcyc=200) maxdisk=2147483648\|a2\|0,1\C,1.6965450391,0.8441244707,0.7627257787\C,1.0171127178,0.1138991245,1.7502024795\C,2.0108838208,0.2173549147,-0.597063632\C,1.9766855726,-1.3073921902,-0.5494067222\C,0.6381909415,-1.7400865195,0.0423117693\C,0.5203362462,-1.298102384,1.5051801407\C,0.3432914526,2.3300556127,0.1759063475\C,-0.9715594258,1.3085122295,2.1985903188\C,-0.4312131864,2.5825588343,2.3838407075\C,0.253671104,3.1380051113,1.3174502722\H,2.9871236566,0.5687422105,-0.9424446794\H,1.2941564979,0.5232298268,-1.3685230375\H,2.7765708387,-1.6687056456,0.1189069286\H,0.5442824762,-2.8263246271,-0.0361904323\H,1.1562418668,-1.9503413791,2.1242587026\H,-0.5047977248,-1.4316187013,1.8723701476\H,-0.4162267271,3.0371043829,3.3700503984\H,0.8789505742,4.0183044441,1.4088698872\H,0.862555413,2.6485287719,-0.721052859\H,-1.4363909718,0.758635157,3.0092443369\C,-1.396250511,0.9038863499,0.8661782884\O,-0.7181933778,1.5229835753,-0.1513155106\O,-2.2663928042,0.1049522315,0.599183947\H,-0.1769064818,-1.2987142524,-0.5475852932\H,2.4235836381,1.5623989137,1.1340125992\H,1.2229567683,0.3669316182,2.786753263\C,2.253161274,-1.9640913721,-1.9437754561\O,2.6216280389,-1.1856195494,-2.8546673194\O,2.0952282737,-3.2059331586,-1.9748283714\|Version=ES64L-G09RevE.01\State=1-A\HF=-765.7140501\|RMSD=6.468e-09\|RMSF=5.066e-06\|Dipole=-1.0062439,4.2957924,4.9202811\|Quadrupole=1.1924641,0.5156911,-1.7081551,14.1260483,15.8754584,-19.1075921\|PG=C01 [X(C12H13O4)]\|@

5g(i) [product]

1\1\GINC-R692\FTS\IRM062X\6-31+G(d,p)\C12H14O4\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc, noeigentest,maxcyc=200) maxdisk=2147483648\|a3\|0,1\C,1.7645866875,0.7955842428,0.878529329\C,0.9290313686,0.0624152883,1.7378228487\C,2.1218094336,0.2623422172,-0.5071024889\C,1.9131746566,-1.2472516357,-0.6104885452\C,0.4915451795,-1.5971571722,-0.1472607374\C,0.3453533179,-1.2808182172,1.3423740803\C,0.6176681023,2.4657055222,0.3111300536\C,-0.9594730278,1.3329296572,2.0666034286\C,-0.3744796551,2.5464134416,2.4428829118\C,0.457199736,3.1516601749,1.5215553807\H,3.1599313198,0.5216434559,-0.7354139722\H,1.5095435689,0.7204082026,-1.2921487979\H,2.6276669262,-1.7826397866,0.0314821202\H,0.2794618278,-2.6559169518,-0.3179442804\H,0.8870881101,-2.0415705421,1.922787653\H,-0.7075086586,-1.3651001969,1.6307547703\H,-0.4513791999,2.9025723999,3.4650935236\H,1.1101269224,3.980985643,1.7655976756\H,1.245727507,2.8471951911,-0.4869638777\H,-1.5488623573,0.7455001656,2.7620046026\C,-1.2613057923,1.0930713568,0.6614475036\O,-0.4417083747,1.7654658627,-0.2097730239\O,-2.1168733967,0.3607421726,0.2205704191\H,-0.2315769787,-1.0156064754,-0.7316766822\H,2.5358547117,1.3893670055,1.3580929116\H,1.077338867,0.2001680595,2.8039362787\C,2.1601405813,-1.7237403181,-2.022450296\O,2.3906619271,-1.0225910228,-2.9778827048\O,2.0951836866,-3.0685409608,-2.1177237155\H,2.2478330034,-3.2996297799,-3.0468673689\|Version=ES64L-G09RevE.01\State=1-A\HF=-766.2692108\|RMSD=7.154e-09\|RMSF=6.631e-06\|Dipole=1.3506001,0.2009485,1.5027936\|Quadrupole=-8.792691,7.0134627,1.7792282,1.120406,-0.917469,5.8126943\|PG=C01 [X(C12H14O4)]\|@

5g(iii) [product]

1\1\GINC-R1369\FTS\IRM062X\6-31+G(d,p)\C13H19N1O2\ROOT\07-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc, noeigentest,maxcyc=200) maxdisk=2147483648\|a3\|0,1\C,1.613140832,0.5007180517,0.7733707576\C,0.5720054754,-0.0716298663,1.5112038734\C,1.8697088355,-0.1096655785,-0.5870354732\C,1.9587665134,-1.6567856888,-0.5472152008\C,0.9814250078,-2.2709741839,0.4903696551\C,-0.1159972745,-1.2731487615,0.908698019\C,0.863491831,2.4197659304,0.1806940234\C,-1.1112052076,1.5416703906,1.6834163673\C,-0.3374469024,2.5847823835,2.2003150133\C,0.7051836085,3.0491607046,1.4189050605\H,2.7830184516,0.2843044286,-1.0406410076\H,1.0463593219,0.1632169672,-1.2559203022\H,2.9802076213,-1.9145694084,-0.245396565\H,1.5349144866,-2.5739910139,1.3855658998\H,-0.8090063576,-1.7241055923,1.6244842054\H,-0.7100902282,-0.9985300616,0.0282835793\H,-0.4600589518,2.9017787947,3.2309965363\H,1.4765138097,3.7115379328,1.7928470805\H,1.6422838637,2.6990809656,-0.52

09774405\H,-1.889350207,1.0629709771,2.267198183\C,-1.2704006451,1.418
8118091,0.2421278972\O,-0.2391660799,1.9605889686,-0.4868786087\O,-2.1
778218069,0.8795273465,-0.3479689431\H,0.5273733312,-3.1818912015,0.08
40722465\H,2.4562167681,0.9230592394,1.3108660092\H,0.5994103707,-0.00
77731109,2.5940790961\N,1.8196084592,-2.1740432277,-1.9145971548\C,2.3
879178498,-3.5022154021,-2.06396757\H,2.3677416157,-3.7872630117,-3.12
00765132\H,3.4294447107,-3.5010987905,-1.7302137034\H,1.8409469412,-4.
2782508298,-1.496139949\C,0.462813986,-2.1462484815,-2.4420885123\H,-0
.2099583465,-2.8720609157,-1.9504090829\H,0.0179967085,-1.1534157103,-
2.3441110761\H,0.4940446077,-2.3919880534,-3.5073754001\Version=ES64L
-G09RevE.01\State=1-A\HF=-711.6544742\RMSD=9.606e-09\RMSF=4.665e-06\Di
pole=1.4062356,-0.0289356,1.2866998\Quadrupole=-6.9802125,4.0902154,2.
8899971,4.2316871,-2.5679604,4.409414\PG=C01 [X(C13H19N1O2)]\@

5g(iv) [product]

1\1\GINC-R1379\FTS\RM062X\6-31+G(d,p)\C13H20N1O2(1+)\ROOT\07-Aug-2017\0
0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,ca
lcf, noeigentest, maxcyc=200) maxdisk=2147483648\la1\1,1\C,1.849491811
9,0.5493363922,1.1916806839\C,0.7436773123,-0.1461038248,1.7147519005\
C,2.8063242943,-0.1491971017,0.2228658393\C,2.3929106233,-1.5515098523
,-0.2606855867\C,1.7589938318,-2.3062146097,0.9062449161\C,0.489919677
8,-1.6104282424,1.4103267681\C,1.0963595137,2.0532912635,0.0667099584\
C,-1.1948540989,0.9679086802,0.8010502393\C,-0.9115113485,2.2517764626
,1.2932982947\C,0.2821206267,2.8239486221,0.9191085516\H,3.745717614,-
0.306522981,0.764901695\H,3.0735535465,0.4971319548,-0.6170784273\H,3.
2962349719,-2.0744321356,-0.5959346075\H,2.5103462305,-2.3125126292,1.
7035663971\H,0.1538870234,-2.0958586233,2.3306724917\H,-0.326850467,-1
.747445053,0.689091635\H,-1.5544541393,2.7063208169,2.0393446023\H,0.6
69758054,3.7329331649,1.3629507903\H,2.0118323998,2.4633045456,-0.3476
736497\H,-2.0492192711,0.3936163042,1.1411037159\C,-0.607593713,0.5350
144463,-0.4322043282\O,0.4780209471,1.2383635286,-0.8597629224\O,-0.93
07667871,-0.4441445093,-1.1063038151\H,1.5653574295,-3.3531163189,0.66
43021916\H,2.3499566856,1.2280094657,1.8761243612\H,0.3281404902,0.222
3542204,2.6457733929\N,1.5025213454,-1.5579718677,-1.4971426243\C,2.13
8009096,-0.8835307293,-2.6654787199\H,1.466357101,-0.9756593426,-3.518
5119479\H,2.2796688645,0.1715843807,-2.4475650509\H,3.0913503664,-1.36
98505881,-2.8827699946\C,1.0936785688,-2.9430234001,-1.8781396186\H,1.
9837982116,-3.5681754113,-1.9762356885\H,0.4229317667,-3.3457192294,-1
.1219305663\H,0.562469552,-2.8925097,-2.827791107\H,0.5906218683,-1.05
75980989,-1.3247497703\Version=ES64L-G09RevE.01\State=1-A\HF=-712.059
9576\RMSD=6.409e-09\RMSF=3.746e-06\Dipole=1.5053553,-0.6640581,0.08466
59\Quadrupole=-5.9299504,6.1084861,-0.1785358,-4.0584916,-8.1069356,9.
360455\PG=C01 [X(C13H20N1O2)]\@

5f(ii) [product]

1\1\GINC-R200\FTS\RM062X\6-31+G(d,p)\C12H13O4(1-)\ROOT\08-Aug-2017\0\0
#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcf
c, noeigentest, maxcyc=200) maxdisk=2147483648\la5\1,1\C,1.5270839146,
0.6320207728,0.2895857532\C,0.7526246672,-0.0757563109,1.2134351328\C,
2.2884593277,-0.0244710557,-0.8378370909\C,1.6873168912,-1.3871657837,
-1.1821563189\C,1.5872007376,-2.2150650026,0.1028913059\C,0.5651973979
,-1.5781753906,1.0476266981\H,3.3491839559,-0.1535222399,-0.584620968\
H,2.2256546578,0.6437427259,-1.7013225258\H,2.3399216638,-1.9090583617
,-1.8922033501\H,2.5701183567,-2.2731935625,0.5914016949\H,0.571439571
2,-2.0908761847,2.0189246463\H,-0.4338383572,-1.7235305879,0.616092411
8\C,3.4454722072,1.563227872,1.6975309921\C,1.7235451913,0.0689567183,
3.0201081547\C,1.7252942971,1.4375230642,3.3392262782\C,2.6146759848,2
.2083693482,2.610938373\H,4.0903205116,2.1071047912,1.0174377471\H,1.0
905057146,-0.6315177626,3.5544439913\H,0.9234211981,1.8590214011,3.933
1089425\H,2.5827471985,3.293848814,2.6469313976\O,2.9126267223,-0.5333
231354,2.6869843497\C,3.783122222,0.1683837315,1.8847973339\O,4.744186
5955,-0.4164509197,1.4263468874\H,1.2577861242,-3.2285167316,-0.143625
8885\H,1.3295748075,1.694213943,0.1918494085\H,-0.1210148992,0.4559483
672,1.5830119824\C,0.2692180814,-1.2667793065,-1.8337829195\O,-0.21349
26571,-0.1089209048,-1.9058392269\O,-0.2438680841,-2.3565123086,-2.176
9761928\Version=ES64L-G09RevE.01\State=1-A\HF=-765.7188217\RMSD=3.331
e-09\RMSF=3.140e-06\Dipole=1.409297,2.2125147,3.8866518\Quadrupole=-6.

7979417,13.1906814,-6.3927398,-4.6540048,-26.1406015,-8.9217986\PG=C01
[X(C12H13O4)]\@

5f(i) [product]

1\1\GINC-R201\FTS\RM062X\6-31+G(d,p)\C12H14O4\ROOT\08-Aug-2017\0\#M06
2X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,no
eigentest,maxcyc=200) maxdisk=2147483648\|a2\|0,1\C,1.5722611458,0.648
5422963,0.29694052\C,0.7822661942,-0.1220099765,1.1646106457\C,2.38815
22323,0.054453037,-0.8415159167\C,1.9954090992,-1.3908570463,-1.148668
3641\C,1.8815983002,-2.1907219578,0.1587353041\C,0.7420158422,-1.63780
11494,1.0158622416\H,3.4610050795,0.0614832252,-0.6230264835\H,2.23101
4269,0.6805781214,-1.7246140034\H,2.7546523914,-1.8573402477,-1.787150
4837\H,2.8367460915,-2.1092858628,0.6891105517\H,0.7473905149,-2.13829
56227,1.9902764787\H,-0.2198426602,-1.8972103947,0.5505677519\C,3.2753
287005,1.5560677113,1.6253015838\C,1.6624181096,0.062568658,3.05016044
8\C,1.6151064375,1.4388389965,3.3123374002\C,2.470734718,2.2170899329,
2.5587416034\H,3.8977091424,2.0982564997,0.9220555813\H,1.0467613675,-
0.641115809,3.5999253305\H,0.81588133,1.8496612644,3.9172687468\H,2.41
48139566,3.3008912195,2.5676725354\O,2.8635267971,-0.513798779,2.71711
93988\C,3.6925515467,0.1862931722,1.8782435572\O,4.6533134212,-0.37832
6016,1.402367696\H,1.7042145191,-3.2481767573,-0.0542030568\H,1.268806
9649,1.6794407507,0.1532507218\H,-0.1498622464,0.3317891873,1.48850682
19\C,0.6911509292,-1.4489215386,-1.916033068\O,0.0066702409,-0.5052571
999,-2.2325344024\O,0.3427542275,-2.7174947393,-2.2211282884\H,-0.4919
076624,-2.6761549753,-2.7127388515\Version=ES64L-G09RevE.01\State=1-A
\HF=-766.2700015\RMSD=5.329e-09\RMSF=3.757e-06\Dipole=-1.4102549,0.429
1993,0.2331495\Quadrupole=-7.2750782,5.6347215,1.6403567,4.9992815,-6.
4752039,5.2452187\PG=C01 [X(C12H14O4)]\@

5f(iii) [product]

1\1\GINC-R215\FTS\RM062X\6-31+G(d,p)\C13H19N1O2\ROOT\08-Aug-2017\0\#M
062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,
noeigentest,maxcyc=200) maxdisk=2147483648\|a1\|0,1\C,1.2815088805,0.7
832820915,0.355696688\C,0.577654531,0.177366812,1.4068118448\C,1.68937
29937,0.0320192966,-0.8951074346\C,1.5045996679,-1.4909451079,-0.81920
77814\C,0.154396376,-1.777349204,-0.1609175335\C,0.1727114172,-1.28849
82234,1.2885594437\H,2.7218891687,0.2748733173,-1.1602666906\H,1.05644
68523,0.395119925,-1.7191002194\H,2.3024789688,-1.915586973,-0.1760122
256\H,-0.0677080156,-2.8466959262,-0.1569147303\H,0.865298654,-1.93306
21689,1.8443645451\H,-0.8141503808,-1.4181499034,1.7441352463\C,3.3395
22915,1.4103494326,1.2297721796\C,1.9525445748,0.0440842795,2.97937031
74\C,2.188725148,1.3873011104,3.3008332366\C,2.9159340308,2.1014303535
,2.3690924446\H,3.8305063516,1.91656289,0.4059562668\H,1.3971088657,-0
.6132862585,3.6400886884\H,1.6501645362,1.8530536306,4.1173297802\H,3.
0245726323,3.1793785411,2.4325065446\O,2.9178942926,-0.6637869357,2.30
61260855\C,3.6242181952,-0.0145536835,1.3237741973\O,4.3788052003,-0.6
493579307,0.622760637\H,-0.6357778828,-1.2765667795,-0.7360573626\H,1.
1491357359,1.8514494629,0.2176268053\H,-0.108985146,0.8152018313,1.954
1663697\N,1.6016999862,-2.0703338412,-2.1666513623\C,2.8777840106,-1.7
381152162,-2.7974713538\H,2.9551794082,-2.2777069985,-3.7442851086\H,2
.9356854707,-0.6726356506,-3.0253898193\H,3.7418955795,-2.008251345,-2
.1641742113\C,1.4534760047,-3.520807936,-2.1427593821\H,2.1701601005,-
4.0062453289,-1.4537370281\H,0.4418004584,-3.809872871,-1.8556249012\H
,1.6291004181,-3.9115646923,-3.1478041765\Version=ES64L-G09RevE.01\St
ate=1-A\HF=-711.6569119\RMSD=5.658e-09\RMSF=4.978e-06\Dipole=-1.272083
,0.9760557,0.6369512\Quadrupole=-7.516717,5.6850103,1.8317067,2.408277
2,-5.4207601,2.9056934\PG=C01 [X(C13H19N1O2)]\@

5f(iv) [product]

1\1\GINC-R219\FTS\RM062X\6-31+G(d,p)\C13H20N1O2(1+)\ROOT\08-Aug-2017\0
\#M062X/6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,cal
cfc,noeigentest,maxcyc=200) maxdisk=2147483648\|a2\|1,1\C,1.1723146445
,0.8630067074,0.3767292125\C,0.528724322,0.204195866,1.4426781343\C,1.
453324332,0.1714409968,-0.9486508552\C,1.3292416883,-1.3397541935,-0.7
92180402\C,-0.021394915,-1.6904236098,-0.1861473475\C,0.021055953,-1.2
334883283,1.2790639201\H,2.4429262558,0.446632604,-1.324947231\H,0.708
0584807,0.5344510309,-1.6698413111\H,2.1228609059,-1.7101653954,-0.136

0838444\H,-0.2179313229,-2.7691371013,-0.2269127808\H,0.6491532727,-1.9440204257,1.8284619708\H,-0.980836331,-1.3019529678,1.7096103666\C,3.3005760869,1.3774498605,1.0968611669\C,2.0212521899,-0.0961026517,2.8443313951\C,2.343912282,1.2074337319,3.2550710288\C,3.0117201402,1.9782893318,2.3309127095\H,3.7389709932,1.9425256935,0.2811093419\H,1.5279715697,-0.7932205358,3.5132966652\H,1.9200734525,1.6073775003,4.1683816701\H,3.1853176362,3.0380847915,2.4831428149\O,2.8932073678,-0.7691932331,2.0160953655\C,3.5231692336,-0.0546828394,1.03722747\O,4.1374369311,-0.6581825107,0.1769767816\H,-0.8298355862,-1.1760657835,-0.718865201\H,1.0498959647,1.9367845714,0.296994859\H,-0.0885510097,0.83157468,2.0762900514\N,1.59495472,-2.0778561166,-2.0977330003\C,0.5863274919,-1.8402424643,-3.1731528574\H,0.8342103736,-2.4750972775,-4.0240519462\H,-0.4072709417,-2.0857790754,-2.8009698135\H,0.6328694272,-0.7941110415,-3.4728637619\C,2.9922878206,-1.8492685559,-2.5998633397\H,3.0348498362,-0.8652073626,-3.0653053985\H,3.6817233409,-1.8872775524,-1.7546620852\H,3.2206421873,-2.6162794101,-3.3399861181\H,1.5332492064,-3.070014934,-1.8490606302\Version=ES64L-G09RevE.01\State=1-A\HF=-712.0491755\IRMSD=8.134e-09\IRMSF=7.418e-06\Dipole=-1.8571125,-0.8909836,-2.3262695\Quadrupole=-15.613289,0.8214461,14.7918429,5.5076934,0.4062018,15.9086696\PG=C01 [X(C13H20N1O2)]\@

5h(ii) [product]

1\1\GINC-R226\FTS\RM062X\6-31+G(d,p)\C12H13O4(1-)\ROOT\08-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,c,noeigentest,maxcyc=200) maxdisk=2147483648\la1\1\C,1.4442314153,0.7114392767,0.2941446509\C,0.7120927438,0.0055046949,1.2501922678\C,1.4843718018,0.1427568899,-1.0932239301\C,1.9992668811,-1.3183443715,-0.9703520996\C,1.112801877,-2.1351706498,-0.0151745739\C,0.0739977555,-1.2709474737,0.7424023756\C,0.3173318551,2.9045716993,0.1099681604\C,-0.9921540413,1.2024047404,1.6470915411\C,-0.4334354948,2.3107754608,2.291687776\C,0.2723599916,3.1816081212,1.4732871613\H,2.1429387479,0.703127027,-1.7587354325\H,3.0213693223,-1.2547488949,-0.5760548821\H,-0.3791639692,-1.8351411589,1.56612994\H,-0.7352937647,-1.0142948243,0.0477981017\H,-0.372441212,2.336032136,3.3730694472\H,0.886527164,3.9743232064,1.8908170075\H,0.9206083395,3.4831043702,-0.5795129335\H,-1.5646277631,0.4484321375,2.1774546645\O,-1.4518792179,1.3324812387,0.3648606418\C,-0.766656804,2.1559780411,-0.5030777312\O,-1.1230697894,2.2010478808,-1.657526625\H,0.5965312797,-2.8911383078,-0.6147841367\H,2.2632259494,1.3502947542,0.6118640605\H,1.0525489539,0.0291615347,2.2822771288\H,0.4867686162,0.1241036098,-1.5533135714\H,1.7362659296,-2.6609717433,0.7184018455\C,2.1433055615,-1.9192284097,-2.4215906944\O,1.3925060593,-2.8754892291,-2.7142879626\O,3.0057718118,-1.3379017568,-3.1182521975\Version=ES64L-G09RevE.01\State=1-A\HF=-765.7110939\IRMSD=3.877e-09\IRMSF=2.546e-06\Dipole=-1.3170348,3.1881314,5.6901121\Quadrupole=5.4747107,-1.5994731,-3.8752376,16.2991247,11.9250784,-18.0547073\PG=C01 [X(C12H13O4)]\@

5h(i) [product]

1\1\GINC-R232\FTS\RM062X\6-31+G(d,p)\C12H14O4\ROOT\08-Aug-2017\0\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcfc,noeigentest,maxcyc=200) maxdisk=2147483648\la1\0,1\C,1.5689241546,0.8634430964,0.4141313419\C,0.9528235154,0.0950792044,1.4170112171\C,1.8664518579,0.3312072169,-0.9792450161\C,1.7344276474,-1.1903921051,-1.0496898712\C,0.4269218283,-1.6352751705,-0.3841725635\C,0.4935880708,-1.3254814514,1.1122833649\C,0.0775401637,2.5752779405,-0.0825454639\C,-0.8773185302,1.0228300065,1.7971860215\C,-0.5225904598,2.3195904351,2.1951390987\C,-0.0252144815,3.1325423398,1.1964650447\H,2.8794600309,0.6366028139,-1.2589356325\H,2.5667849047,-1.6674248508,-0.5092642045\H,1.2096216018,-2.0119879883,1.5846683622\H,-0.4787836357,-1.5382528986,1.5698634227\H,-0.4639305622,2.5682424122,3.2479310228\H,0.4187185354,4.09880537,1.4136416412\H,0.5523466817,3.1053417757,-0.9008590641\H,-1.2957605883,0.308894274,2.4984681453\O,-1.4080702986,0.8292123051,0.5460176419\C,-0.8658053802,1.5443153963,-0.4922408049\O,-1.1739851244,1.2534006858,-1.6255551415\H,-0.4121770696,-1.1062640752,-0.8522745168\H,2.2216483353,1.6624043948,0.7489872573\H,1.3070479024,0.2566476384,2.4311325587\H,1.2036075562,0.7566532613,-1.7410404648\H,0.2683804929,-2.706756461,-0.5299335484\C,1.8549720091,-1.6640579554,-2.480424779\O,2.13

31098526,-0.9745486884,-3.4306248159\O,1.6443530266,-2.9928482935,-2.5
955395545\H,1.7514079627,-3.2185506291,-3.5323106992\Version=ES64L-GO
9RevE.01\State=1-A\HF=-766.2675685\RMSD=4.647e-09\RMSF=2.370e-06\Dipol
e=0.9264871,-0.079713,2.0377058\Quadrupole=-6.1562819,6.519847,-0.3635
651,2.0491279,-1.9244354,6.235672\PG=C01 [X(C12H14O4)]\@

5h(iii) [product]

1\1\GINC-R174\FTS\RM062X\6-31+G(d,p)\C13H19N1O2\ROOT\08-Aug-2017\0\#M
062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,calcf,
noeigentest,maxcyc=200) maxdisk=2147483648\la5\0,1\1C,1.6593962988,0.5
247830747,0.6852812185\C,0.6605718601,-0.0700395604,1.462543631\C,1.87
90414637,-0.0439137682,-0.689437787\C,2.1091275538,-1.5833071608,-0.60
61496101\C,1.0688963058,-2.252399681,0.3282793495\C,-0.0099211905,-1.2
757954983,0.8305093921\C,0.9111464272,2.7665426585,0.2879859603\C,-0.9
299021525,1.3065077775,1.4789982499\C,-0.3864778948,2.3523447921,2.234
6636849\C,0.588001303,3.1044143628,1.6037323155\H,2.7193868369,0.44648
54707,-1.1887680977\H,0.9976770353,0.1296962894,-1.3186305867\H,3.1049
470251,-1.7411538416,-0.1756212408\H,1.5846457248,-2.6727989943,1.1976
636021\H,-0.6707171464,-1.7734286646,1.5470627347\H,-0.633331004,-0.95
21983623,-0.0132010303\H,-0.5848468104,2.4120371925,3.2979634601\H,1.1
806820279,3.8347011466,2.1453996812\H,1.7210481585,3.2503341134,-0.245
9822369\H,-1.7093560759,0.658180298,1.865933983\O,-1.0642785069,1.454
4369137,0.1238929126\C,-0.0976848821,2.1540340711,-0.560028604\O,-0.14
56242488,2.1785787076,-1.7682706798\H,0.6106590599,-3.0963458715,-0.19
52357893\H,2.4863231559,1.032063142,1.1699712312\H,0.7866539756,-0.082
4946958,2.5410393958\N,2.1449014602,-2.2455553416,-1.9129090672\C,0.93
99340941,-2.0761573126,-2.7114627693\H,0.9623130868,-2.7880882639,-3.5
421614061\H,0.0502413239,-2.2891930295,-2.1123368749\H,0.8318365783,-1
.0636937698,-3.13610432\C,3.3251233947,-1.9118073784,-2.69052769\H,3.3
295810382,-0.8710443287,-3.0607839504\H,4.223170806,-2.0696401865,-2.0
85855461\H,3.3804579181,-2.5732603009,-3.5606036008\Version=ES64L-G09
RevE.01\State=1-A\HF=-711.6543339\RMSD=3.690e-09\RMSF=3.240e-06\Dipole
=0.6397634,-0.2400953,1.701674\Quadrupole=0.533604,-3.2666977,2.733093
7,5.6014178,-4.5466869,6.1692194\PG=C01 [X(C13H19N1O2)]\@

5h(iv) [product]

1\1\GINC-R172\FTS\RM062X\6-31+G(d,p)\C13H20N1O2(1+)\ROOT\08-Aug-2017\0
\#M062X\6-31+G** SCF=Tight IOP(2/17=4) INT(grid=ultrafine) OPT(TS,cal
cfc,noeigentest,maxcyc=200) maxdisk=2147483648\la6\1,1\1C,1.7896470539
.0.8180555356,0.8070978473\C,1.016878467,-0.0469296384,1.6026877568\C,
2.6090362872,0.3524678747,-0.3855334149\C,2.4947705628,-1.1409234544,-
0.7590351522\C,2.1953234744,-1.9796377301,0.4800020398\C,0.9313591853,
-1.5181612919,1.2095833291\C,0.2496792261,2.3877826683,-0.1088476479\C
,-0.9218700893,0.528553178,1.3440286007\C,-0.9767145234,1.8423897608,1
.8469579995\C,-0.365641191,2.8075642168,1.0808651727\H,3.6575769955,0.
5236899425,-0.1130059699\H,2.4302741078,0.987121646,-1.2592903577\H,3.
4468038537,-1.4710129653,-1.1883344429\H,3.0604324702,-1.8536474966,1.
1411110642\H,0.7864905419,-2.1250291772,2.1068169696\H,0.0556472863,-1
.6969654136,0.5723231198\H,-1.3370756665,2.0225955529,2.8526391028\H,-
0.2428384297,3.8260514255,1.432827966\H,0.8515649181,3.058378785,-0.71
19263182\H,-1.4377623708,-0.2882752166,1.8383528974\O,-0.9577750466,0.
353089243,-0.0224625703\C,-0.2234124888,1.2080468151,-0.7771465809\O,0.
0219989926,0.8735469966,-1.9366850876\H,2.1499050615,-3.0448465949,0.
2402854509\H,2.1932083798,1.7035990236,1.2857079763\H,1.0280858668,0.1
53772457,2.6689662947\N,1.4966129079,-1.344959537,-1.8979608892\C,2.09
81666718,-0.9268909294,-3.2022492459\H,1.3092729405,-0.9055804023,-3.9
536988509\H,2.5200726982,0.0711844527,-3.1054904033\H,2.8720252095,-1.
6458738368,-3.4764470408\C,0.9681499425,-2.7312516152,-2.025294581\H,1
.8046527263,-3.4234674883,-2.1395206757\H,0.3798695103,-2.9906999169,-
1.147965004\H,0.3336456629,-2.7705242102,-2.9106014898\H,0.6974188051,
-0.675695659,-1.7778528644\Version=ES64L-G09RevE.01\State=1-A\HF=-712
.0592349\RMSD=9.354e-09\RMSF=1.958e-06\Dipole=1.2997268,-1.168653,0.07
24203\Quadrupole=-7.2973242,4.7804238,2.5169005,-3.1993905,-9.2378285,
10.8792723\PG=C01 [X(C13H20N1O2)]\@