

## Electronic Supplementary Information

### Computational Design of pH-Switchable Control Agents for Nitroxide Mediated Polymerization

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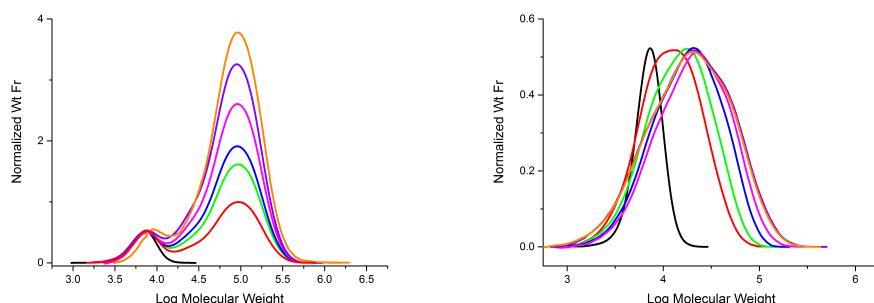
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## Appendix 1. Preliminary Experimental Results

To establish whether or not the presence of base could promote an otherwise stable alkoxyamine to undergo sufficient dissociation to sustain a polymerization, a standard nitroxide mediated polymerization (NMP) of styrene was first performed using (protonated) 4-carboxyl TEMPO at 120°C (full conditions below). The resulting polymeric alkoxyamine was characterised, confirming that a narrow molecular weight distribution polymer was obtained (dispersity = 1.12), and hence the NMP was successful. This polymeric species was then used in 2 otherwise identical chain extension experiments. A stock solution of the polymeric alkoxyamine in the presence of bulk styrene monomer and *tert*-butyl hydroperoxide was prepared and split into two samples for polymerization at 100°C. To one of the samples, 1.5 equivalents of base (1,8-Diazabicyclo[5.4.0]undec-7-ene) was added, the other was base-free. The amount of base required to fully deprotonate the carboxylic acid was determined by repeating the experiments of Ref 1 with DBU and observing convergence of the pH switch on kinetics and thermodynamics with respect to amount of added base.

Each solution was heated to 100°C and samples were taken periodically and their molecular weight distribution analysed by size-exclusion chromatography (SEC). Figure S1 shows the development of the molecular weight distributions as a function of polymerization time for the two samples. It is clear that in the polymerization without base, the initial polymeric alkoxyamine remains intact and an independent thermal polymerization occurs. In contrast, when base is present, the entire molecular weight distribution shifts to higher molecular weights, confirming that homolysis is occurring. The polymerization is not controlled, suggesting that the temperature could be lowered further and/or concentrations of the various species should be optimized. Nonetheless, the shift in the molecular weight distribution is unambiguous in demonstrating homolysis of the polymeric alkoxyamine at 100°C in the presence of base, which is in stark contrast to its stability in the absence of base. Together with our earlier small molecule measurements of pH switching in this system,<sup>1</sup> this clearly demonstrates that pH switching of NMP is possible. At the same time, for this particular system, we find that even when “switched on” the temperatures required to sustain a polymerization remain too high to be synthetically useful.

**Figure S1. pH-switching NMP**



The first graph shows the initial polymeric alkoxyamine (black) and samples taken at 10 minute intervals after polymerization at 100°C in the presence of bulk styrene and BHT; the second shows the identical experiment but with 1.5 equivalents of base (DBU) included. [Red = 10; green = 20, blue = 30, pink = 40, purple = 50, orange = 60 minutes.]

<sup>1</sup> M. Klinska, L. M. Smith, G. Gryn'ova, M. G. Banwell and M. L. Coote, *Chem. Sci.*, 2015, **6**, 5623.

## Detailed Experimental Methods

**Materials.** Styrene (99%, Sigma-Aldrich) was passed through a column of basic alumina to remove the inhibitor. 4-carboxy-TEMPO (97%), azobisisobutyronitrile (AIBN) and *tert*-butyl hydroperoxide solution (BHP) (~5-6M in decane, Aldrich), 1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU, Aldrich, 98%) and tetrahydrofuran (THF) for SEC analysis (Merck LiChrosolv<sup>®</sup>) were used as received.

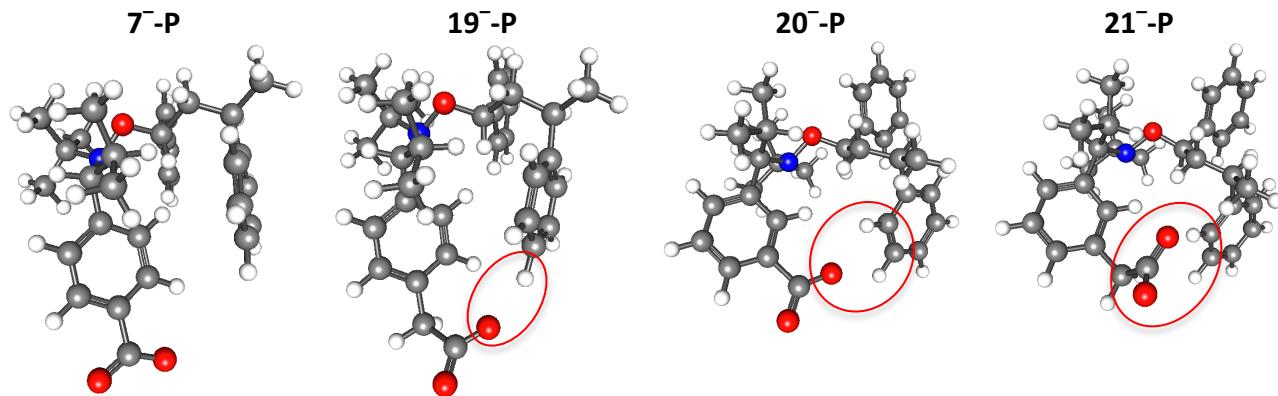
**Synthesis of 4-carboxy-TEMPO polystyrene.** AIBN (12 mg) and 4-carboxy-TEMPO (26 mg) were dissolved into 12 mL of styrene. The sample was then subjected to three freeze-pump-thaw cycles to degas the solution and then the sample was heated to 120°C for ~4 hours. After the end of this time the polymer was precipitated into methanol and dried under vacuum.

**Chain Extension of 4-carboxy-TEMPO polystyrene in the presence of *tert*-butyl hydroperoxide (BHP) at 100°C.** 4-carboxy-TEMPO polystyrene (as above, 138.8 mg) was dissolved into 12 mL of styrene. BHP (5 - 6M solution in dioxane) (80 mM, 160µL) was added to this solution. The solution was then divided into two 6mL portions and 30 µL of DBU (~1.5 eq relative to 4-carboxy-TEMPO-styrene) was added to one portion. Both samples were then degassed via three freeze-pump-thaw cycles and then heated to 100°C. Samples (~1mL) were removed from each vessel at 10-minute intervals and precipitated into methanol. The methanol was then decanted from these samples and they were dried under vacuum prior to SEC analysis.

**SEC Analysis.** The molecular weight distributions of the samples were determined using a Viscotek GPC Max size exclusion chromatography system fitted with a Viscotek TDA 305 triple detector array consisting of a differential viscometer (DV); right angle laser-light scattering (RALLS); low angle laser-light scattering (LALLS); and refractive index detectors. The column set consisted of a Viscotek TGuard Organic Guard Column (10x4.6mm) and two Viscotek LT5000L Mixed Medium Organic Columns (300x7.8 mm). The system was fitted with an online solvent degasser system and eluent (THF) flowrate was set to 1mL/min and columns were held at 30°C. Calibration was carried out using Viscotek PolyCAL<sup>TM</sup> polystyrene standards with M<sub>w</sub> = 98,251 and M<sub>n</sub> = 96,722 and M<sub>w</sub> = 231,820 and M<sub>n</sub> = 102,977 using OmniSEC software version 4.6.1.354.

## Appendix S2 Detailed Computational Results

**Figure S2. Intramolecular H-bonding**



Intramolecular bonding in the deprotonated alkoxyamines of nitroxides **7** and **19-21**.

**Table S1. Calculated energetics of the studied NO–C bond homolysis at temperature *T* in the gas phase and bulk styrene solution.**

Nitroxide <sup>a</sup>	$\Delta H_{gas}^0$	$\Delta H_{gas}^T$	$\Delta G_{gas}^T$	$\Delta G_{soln}^T$	$\log K$
25 °C					
TEMPO	183.378	185.970	119.038	99.266	17.4
<b>12</b>	185.932	188.481	121.119	101.013	17.7
<b>12</b> <sup>-</sup>	167.213	169.638	101.979	88.357	15.5
<b>18</b>	170.211	173.549	98.020	79.628	14.0
<b>18</b> <sup>-</sup>	166.193	169.628	99.562	68.200	11.9
<b>18</b> <sup>2-</sup>	210.612	214.345	138.156	68.804	12.1
<b>7</b>	174.077	177.030	102.422	78.967	13.8
<b>7</b> <sup>-</sup>	168.425	171.385	96.935	75.363	13.2
<b>17</b>	165.568	168.207	95.222	73.818	12.9
<b>17</b> <sup>-</sup>	133.294	135.906	64.300	60.218	10.5
<b>14</b>	171.448	173.847	105.797	88.117	15.4
<b>14</b> <sup>-</sup>	150.425	153.153	81.025	61.838	10.8
<b>15</b>	181.568	184.300	114.422	96.617	16.9
<b>15</b> <sup>-</sup>	164.291	166.899	99.584	88.431	15.5
<b>13</b>	174.968	177.747	112.529	98.154	17.2
<b>13</b> <sup>-</sup>	166.673	169.173	105.329	92.168	16.1
<b>13</b> <sup>2-</sup>	163.232	166.462	96.377	80.203	14.1
<b>16</b>	175.517	178.248	110.999	89.595	15.7
<b>16</b> <sup>-</sup>	157.274	160.085	91.499	76.204	13.4
<b>19</b>	170.311	173.229	99.209	75.797	13.3
<b>19</b> <sup>-</sup>	183.533	187.318	105.975	85.701	15.0
<b>20</b>	163.926	166.816	95.712	72.384	12.7
<b>20</b> <sup>-</sup>	178.805	181.917	107.931	70.837	12.4
<b>21</b>	162.342	165.100	93.122	71.969	12.6
<b>21</b> <sup>-</sup>	176.941	180.262	105.731	70.562	12.4
<b>22</b>	162.619	165.653	92.820	68.905	12.1
<b>22</b> <sup>-</sup>	157.382	160.233	88.923	64.716	11.3
<b>23</b>	162.657	165.566	93.804	69.472	12.2
<b>23</b> <sup>-</sup>	162.212	165.341	89.032	64.532	11.3

60 °C

TEMPO	183.378	185.972	111.184	92.649	14.5
<b>12</b>	185.932	188.496	113.214	94.345	14.8
<b>12<sup>-</sup></b>	167.213	169.634	94.039	81.655	12.8
<b>18</b>	170.211	173.562	89.155	72.002	11.3
<b>18<sup>-</sup></b>	166.193	169.705	91.336	61.212	9.6
<b>18<sup>2-</sup></b>	210.612	214.400	129.212	61.098	9.6
<b>7</b>	174.077	177.023	93.666	71.450	11.2
<b>7<sup>-</sup></b>	168.425	171.378	88.198	67.864	10.6
<b>17</b>	165.568	168.226	86.655	66.489	10.4
<b>17<sup>-</sup></b>	133.294	135.885	55.898	53.053	8.3
<b>14</b>	171.448	173.836	97.812	81.370	12.8
<b>14<sup>-</sup></b>	150.425	153.143	72.560	54.612	8.6
<b>15</b>	181.568	184.314	106.221	89.653	14.1
<b>15<sup>-</sup></b>	164.291	166.907	91.684	81.769	12.8
<b>13</b>	174.968	177.783	104.874	91.737	14.4
<b>13<sup>-</sup></b>	166.673	169.179	97.837	85.913	13.5
<b>13<sup>2-</sup></b>	163.232	166.506	88.150	73.214	11.5
<b>16</b>	175.517	178.297	103.104	82.938	13.0
<b>16<sup>-</sup></b>	157.274	160.132	83.448	69.390	10.9
<b>19</b>	170.311	173.220	90.523	68.348	10.7
<b>19<sup>-</sup></b>	183.533	187.344	96.428	77.391	12.1
<b>20</b>	163.926	166.832	87.367	65.277	10.2
<b>20<sup>-</sup></b>	178.805	181.929	99.248	63.392	9.9
<b>21</b>	162.342	165.077	84.676	64.761	10.2
<b>21<sup>-</sup></b>	176.941	180.315	96.982	63.050	9.9
<b>22</b>	162.619	165.678	84.271	61.595	9.7
<b>22<sup>-</sup></b>	157.382	160.244	80.554	57.584	9.0
<b>23</b>	162.657	165.585	85.382	62.287	9.8
<b>23<sup>-</sup></b>	162.212	165.361	80.075	56.813	8.9

100 °C

TEMPO	183.378	185.910	102.211	85.129	11.9
<b>12</b>	185.932	188.448	104.181	86.764	12.1
<b>12<sup>-</sup></b>	167.213	169.564	84.970	74.038	10.4
<b>18</b>	170.211	173.506	79.028	63.326	8.9
<b>18<sup>-</sup></b>	166.193	169.713	81.930	53.258	7.5
<b>18<sup>2-</sup></b>	210.612	214.386	118.989	52.326	7.3
<b>7</b>	174.077	189.135	82.894	62.130	8.7
<b>7<sup>-</sup></b>	168.425	183.489	77.447	58.566	8.2
<b>17</b>	165.568	168.182	76.867	58.153	8.1
<b>17<sup>-</sup></b>	133.294	135.792	46.303	44.911	6.3
<b>14</b>	171.448	173.763	88.691	73.701	10.3
<b>14<sup>-</sup></b>	150.425	153.071	62.892	46.396	6.5
<b>15</b>	181.568	184.263	96.851	81.735	11.4
<b>15<sup>-</sup></b>	164.291	166.849	82.659	74.196	10.4
<b>13</b>	174.968	177.755	96.125	84.440	11.8
<b>13<sup>-</sup></b>	166.673	169.118	89.278	78.806	11.0
<b>13<sup>2-</sup></b>	163.232	166.480	78.747	65.263	9.1
<b>16</b>	175.517	178.285	94.080	75.366	10.5
<b>16<sup>-</sup></b>	157.274	160.117	74.245	61.640	8.6
<b>19</b>	170.311	173.146	80.601	59.879	8.4
<b>19<sup>-</sup></b>	183.533	187.306	85.517	67.933	9.5
<b>20</b>	163.926	166.783	77.833	57.194	8.0
<b>20<sup>-</sup></b>	178.805	181.875	89.327	54.923	7.7

<b>21</b>	162.342	164.987	75.031	56.568	7.9
<b>21<sup>-</sup></b>	176.941	180.307	86.980	54.501	7.6
<b>22</b>	162.619	165.640	74.502	53.278	7.5
<b>22<sup>-</sup></b>	157.382	160.191	70.992	49.475	6.9
<b>23</b>	162.657	165.540	75.758	54.115	7.6
<b>23<sup>-</sup></b>	162.212	165.320	69.841	48.031	6.7
120 °C					
TEMPO	183.378	185.854	97.728	81.385	10.8
<b>12</b>	185.932	188.399	99.667	82.990	11.0
<b>12<sup>-</sup></b>	167.213	169.504	80.439	70.247	9.3
<b>18</b>	170.211	173.452	73.967	59.006	7.8
<b>18<sup>-</sup></b>	166.193	169.688	77.227	49.295	6.5
<b>18<sup>2-</sup></b>	210.612	214.350	113.879	47.956	6.4
<b>7</b>	174.077	176.891	78.669	58.644	7.8
<b>7<sup>-</sup></b>	168.425	171.246	73.232	55.090	7.3
<b>17</b>	165.568	168.135	71.976	54.002	7.2
<b>17<sup>-</sup></b>	133.294	135.720	41.510	40.858	5.4
<b>14</b>	171.448	173.704	84.135	69.884	9.3
<b>14<sup>-</sup></b>	150.425	153.013	58.062	42.305	5.6
<b>15</b>	181.568	184.213	92.169	77.793	10.3
<b>15<sup>-</sup></b>	164.291	166.795	78.150	70.427	9.4
<b>13</b>	174.968	177.715	91.753	80.807	10.7
<b>13<sup>-</sup></b>	166.673	169.062	85.002	75.270	10.0
<b>13<sup>2-</sup></b>	163.232	166.439	74.048	61.304	8.1
<b>16</b>	175.517	178.253	89.570	71.596	9.5
<b>16<sup>-</sup></b>	157.274	160.083	69.645	57.780	7.7
<b>19</b>	170.311	173.086	75.644	55.662	7.4
<b>19<sup>-</sup></b>	183.533	187.261	80.065	63.220	8.4
<b>20</b>	163.926	166.734	73.068	53.169	7.1
<b>20<sup>-</sup></b>	178.805	181.823	84.370	50.706	6.7
<b>21</b>	162.342	164.918	70.213	52.490	7.0
<b>21<sup>-</sup></b>	176.941	180.277	81.981	50.241	6.7
<b>22</b>	162.619	165.596	69.621	49.136	6.5
<b>22<sup>-</sup></b>	157.382	160.139	66.214	45.437	6.0
<b>23</b>	162.657	165.493	70.949	50.046	6.6
<b>23<sup>-</sup></b>	162.212	165.276	64.726	43.656	5.8

<sup>a</sup> See main text for the structures of the nitroxide radicals.

**Table S2. Electronic energies, Gibbs free energies in the gas phase and of solvation at 25 °C.**

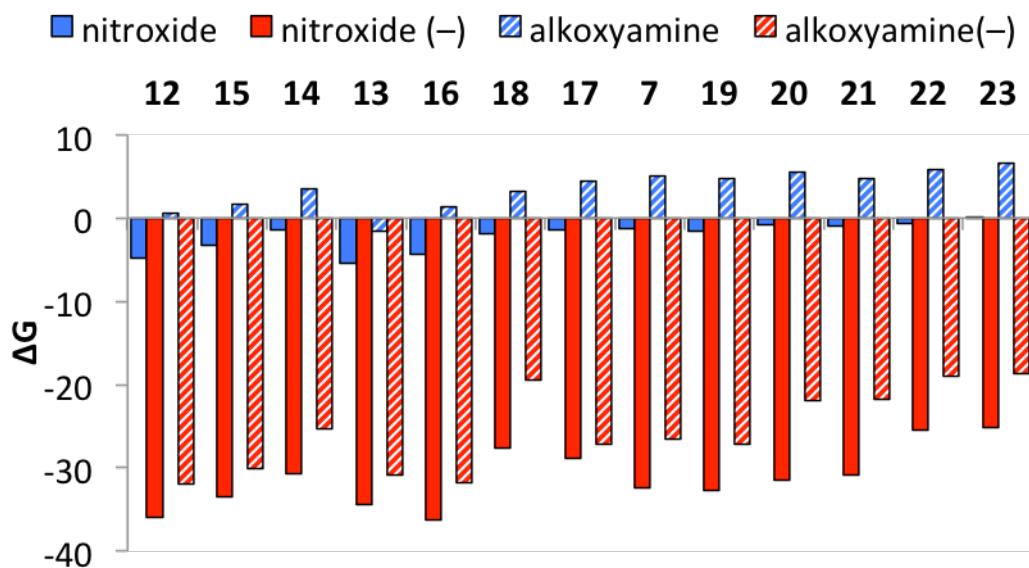
Species <sup>a</sup>	Raw $E_e$ , Hartrees		$E_{ONIOM}^b$ , Hartrees	ZPVE, Hartrees	$G_{gas}$ , Hartrees	$\Delta G_{solv}^c$ , kcal mol <sup>-1</sup>
	M06-2X/6-31+G(d)	G3(MP2,CC)(+)				
P• (core)	-156.49003	-156.36609				
P•	-619.63643		-619.51249	0.27338	-619.28404	-1.19
TEMPO	-483.50459	-483.13966	-483.13966	0.25583	-482.92076	-2.84
TEMPO-P (core)	-640.05774	-639.57231				
TEMPO-P	-1103.21391		-1102.72848	0.53570	-1102.25015	2.59
<b>12</b>	-672.01816	-671.52675	-671.52675	0.27033	-671.29836	-4.88
<b>12-P (core)</b>	-828.57222	-827.96032				
<b>12-P</b>	-1291.72856		-1291.11667	0.55032	-1290.62854	0.63
<b>12<sup>-</sup></b>	-671.47577	-670.97664	-670.97664	0.25679	-670.76274	-35.88

<b>12<sup>-</sup>-P (core)</b>	-828.02251	-827.40310				
<b>12<sup>-</sup>-P</b>	-1291.17850		-1290.55910	0.53645	-1290.08562	-31.92
<b>18 (core)</b>	-777.22161	-776.60321				
<b>18</b>	-1052.29513		-1051.67674	0.29960	-1051.42278	-1.90
<b>18<sup>-</sup>-P (core)</b>	-933.78212	-933.04000				
<b>18-P</b>	-1672.00334		-1671.26122	0.58014	-1670.74416	3.20
<b>18<sup>-</sup> (core)</b>	-776.70002	-776.07452				
<b>18<sup>-</sup></b>	-1051.77370		-1051.14821	0.28799	-1050.90459	-27.66
<b>18<sup>-</sup>-P (core)</b>	-933.25312	-932.50502				
<b>18<sup>-</sup>-P</b>	-1671.47942		-1670.73133	0.56870	-1670.22656	-19.46
<b>18<sup>2-</sup> (core)</b>	-775.98937	-775.35738				
<b>18<sup>2-</sup></b>	-1051.06702		-1050.43503	0.27423	-1050.20566	-101.34
<b>18<sup>2-</sup>-P (core)</b>	-932.53548	-931.78367				
<b>18<sup>2-</sup>-P</b>	-1670.78594		-1670.03414	0.55400	-1669.54233	-84.06
<b>7 (core)</b>	-629.10378	-628.60678				
<b>7</b>	-864.88282		-864.38582	0.34121	-864.09465	-1.25
<b>7-P (core)</b>	-785.66713	-785.04867				
<b>7-P</b>	-1484.58968		-1483.97122	0.62120	-1483.41771	5.06
<b>7<sup>-</sup> (core)</b>	-628.56271	-628.05799				
<b>7<sup>-</sup></b>	-864.34041		-863.83569	0.32797	-863.55728	-32.40
<b>7<sup>-</sup>-P (core)</b>	-785.12214	-784.49631				
<b>7<sup>-</sup>-P</b>	-1484.04474		-1483.41890	0.60792	-1482.87825	-26.54
<b>17 (core)</b>	-437.43299	-437.13138				
<b>17</b>	-864.87803		-864.57643	0.34175	-864.28465	-1.46
<b>17-P (core)</b>	-593.99012	-593.56648				
<b>17-P</b>	-1484.58238		-1484.15873	0.62188	-1483.60496	4.36
<b>17<sup>-</sup> (core)</b>	-436.88734	-436.57802				
<b>17<sup>-</sup></b>	-864.33929		-864.02997	0.32864	-863.75138	-28.88
<b>17<sup>-</sup>-P (core)</b>	-593.43993	-593.00928				
<b>17<sup>-</sup>-P</b>	-1484.03010		-1483.59945	0.60824	-1483.05992	-27.20
<b>14 (core)</b>	-475.52756	-475.18433				
<b>14</b>	-789.89650		-789.55328	0.35377	-789.24638	-1.44
<b>14-P (core)</b>	-632.08780	-631.62351				
<b>14-P</b>	-1409.60170		-1409.13741	0.63349	-1408.57072	3.49
<b>14<sup>-</sup> (core)</b>	-474.98952	-474.63869				
<b>14<sup>-</sup></b>	-789.35881		-789.00798	0.34037	-788.71405	-30.64
<b>14<sup>-</sup>-P (core)</b>	-631.53880	-631.06715				
<b>14<sup>-</sup>-P</b>	-1409.05594		-1408.58429	0.62029	-1408.02895	-25.35
<b>15 (core)</b>	-627.90858	-627.40047				
<b>15</b>	-785.10758		-784.59947	0.26373	-784.38134	-3.35
<b>15-P (core)</b>	-784.46834	-783.83879				
<b>15-P</b>	-1404.81716		-1404.18761	0.54360	-1403.70896	1.61
<b>15<sup>-</sup> (core)</b>	-627.37117	-626.85540				
<b>15<sup>-</sup></b>	-784.56864		-784.05288	0.25050	-783.84749	-33.53
<b>15<sup>-</sup>-P (core)</b>	-783.92352	-783.28641				
<b>15<sup>-</sup>-P</b>	-1404.27128		-1403.63417	0.53010	-1403.16947	-30.16
<b>13 (core)</b>	-664.03988	-663.57030				
<b>13</b>	-821.23999		-820.77041	0.25583	-820.55981	-5.43
<b>13<sup>-</sup> (core)</b>	-663.50942	-663.03167				
<b>13<sup>-</sup></b>	-820.70591		-820.22817	0.24292	-820.03062	-34.34
<b>13<sup>2-</sup> (core)</b>	-662.85769	-662.37199				
<b>13<sup>2-</sup></b>	-820.05765		-819.57195	0.22991	-819.38667	-101.51
<b>13-P (core)</b>	-820.60258	-820.01157				

<b>13-P</b>	-1440.94730		-1440.35629	0.53595	-1439.88671	-1.59
<b>13<sup>-</sup>-P (core)</b>	-820.05968	-819.46119				
<b>13<sup>-</sup>-P</b>	-1440.40871		-1439.81022	0.52237	-1439.35478	-30.79
<b>13<sup>2-</sup>-P(core)</b>	-819.41066	-818.80433				
<b>13<sup>2-</sup>-P</b>	-1439.75929		-1439.15296	0.50965	-1438.70742	-97.24
<b>16 (core)</b>	-514.82805	-514.45443	0.37362	0.16046		
<b>16</b>	-632.72446		-632.35085	0.24160	-632.15126	-4.40
<b>16-P (core)</b>	-671.38721	-670.89329	0.49391	0.25939		
<b>16-P</b>	-1252.43101		-1251.93710	0.52189	-1251.47758	1.42
<b>16<sup>-</sup> (core)</b>	-514.28187	-513.90041	0.38146	0.14717		
<b>16<sup>-</sup></b>	-632.17842		-631.79696	0.22828	-631.61064	-36.18
<b>16<sup>-</sup>-P (core)</b>	-670.83568	-670.33388	0.50180	0.24575		
<b>16<sup>-</sup>-P</b>	-1251.87790		-1251.37609	0.50840	-1250.92954	-31.82
<b>19 (core)</b>	-668.39348	-667.86719	0.52629	0.20371		
<b>19</b>	-904.17229		-903.64600	0.36851	-903.33072	-1.62
<b>19-P (core)</b>	-824.95607	-824.30843	0.64764	0.30206		
<b>19-P</b>	-1523.87755		-1523.22991	0.64845	-1522.65256	4.68
<b>19<sup>-</sup> (core)</b>	-667.85129	-667.31675	0.53454	0.19045		
<b>19<sup>-</sup></b>	-903.62913		-903.09458	0.35528	-902.79231	-32.65
<b>19<sup>-</sup>-P (core)</b>	-824.40844	-823.75267	0.65577	0.28900		
<b>19<sup>-</sup>-P</b>	-1523.33970		-1522.68394	0.63562	-1522.11671	-27.10
<b>20 (core)</b>	-629.10409	-628.60725	0.49684	0.17666		
<b>20</b>	-864.88301		-864.38617	0.34129	-864.09489	-0.83
<b>20-P (core)</b>	-785.66567	-785.04743	0.61824	0.27493		
<b>20-P</b>	-1484.58590		-1483.96767	0.62124	-1483.41539	5.45
<b>20<sup>-</sup> (core)</b>	-628.56461	-628.06021	0.50441	0.16333		
<b>20<sup>-</sup></b>	-864.34258		-863.83817	0.32808	-863.55962	-31.54
<b>20<sup>-</sup>-P (core)</b>	-785.12213	-784.49593	0.62619	0.26174		
<b>20<sup>-</sup>-P</b>	-1484.05119		-1483.42499	0.60769	-1482.88477	-21.97
<b>21 (core)</b>	-668.39375	-667.86802	0.52573	0.20398		
<b>21</b>	-904.17261		-903.64688	0.36871	-903.33198	-1.03
<b>21-P (core)</b>	-824.95530	-824.30709	0.64821	0.30230		
<b>21-P</b>	-1523.87545		-1523.22724	0.64813	-1522.65149	4.73
<b>21<sup>-</sup> (core)</b>	-667.85569	-667.32158	0.53411	0.19055		
<b>21<sup>-</sup></b>	-903.63547		-903.10136	0.35538	-902.79717	-30.87
<b>21<sup>-</sup>-P (core)</b>	-824.41057	-823.75461	0.65596	0.28901		
<b>21<sup>-</sup>-P</b>	-1523.34386		-1522.68790	0.63542	-1522.12148	-21.76
<b>22 (core)</b>	-616.55264	-616.06536	0.48728	0.18544		
<b>22</b>	-852.33154		-851.84426	0.35009	-851.54571	-0.61
<b>22-P (core)</b>	-773.11419	-772.50522	0.60897	0.28372		
<b>22-P</b>	-1472.03440		-1471.42543	0.63021	-1470.86511	5.81
<b>22<sup>-</sup> (core)</b>	-692.41783	-691.89877	0.51906	0.19608		
<b>22<sup>-</sup></b>	-928.19550		-927.67645	0.36096	-927.36934	-25.50
<b>22<sup>-</sup>-P (core)</b>	-848.97683	-848.33597	0.64087	0.29470		
<b>22<sup>-</sup>-P</b>	-1547.89623		-1547.25536	0.64081	-1546.68725	-19.01
<b>23 (core)</b>	-655.84730	-655.32976	0.51754	0.21244		
<b>23</b>	-891.62603		-891.10849	0.37721	-890.78499	0.09
<b>23-P (core)</b>	-812.40933	-811.76983	0.63950	0.31103		
<b>23-P</b>	-1511.32901		-1510.68951	0.65717	-1510.10476	6.61
<b>23<sup>-</sup> (core)</b>	-731.71227	-731.16333	0.54894	0.22306		
<b>23<sup>-</sup></b>	-967.48999		-966.94105	0.38795	-966.60838	-25.22
<b>23<sup>-</sup>-P (core)</b>	-888.27169	-887.60107	0.67062	0.32167		
<b>23<sup>-</sup>-P</b>	-1587.19256		-1586.52195	0.66795	-1585.92633	-18.66

<sup>a</sup> P• = •CH(Ph)CH<sub>2</sub>CH(Ph)CH<sub>3</sub> dimeric propagating styryl radical, see main text for the structures of the nitroxide radicals; <sup>b</sup> Electronic energy, used to calculate the free energy; <sup>c</sup> Free energy of solvation in toluene, calculated using UAKS-CPCM/B3LYP/6-31+G(d) method.

**Figure S3. Computed free energies of solvation (in kcal mol<sup>-1</sup>) in toluene of the investigated nitroxides and their corresponding alkoxyamines (with dimeric propagating styryl radical) in neutral and (singly) deprotonated states.**



**Table S3. Gas-phase entropies and thermal corrections.**

Species <sup>a</sup>	<i>S<sub>gas</sub></i> , J mol <sup>-1</sup> K <sup>-1</sup>				TC, Hartrees			
	25 °C	60 °C	100 °C	120 °C	25 °C	60 °C	100 °C	120 °C
P• (core)	302.5801	312.6490	323.8963	329.4239	0.00639	0.00759	0.00910	0.00990
P•	535.5003	565.7451	600.2484	617.4284	0.01588	0.01949	0.02410	0.02660
TEMPO	441.8278	467.2206	495.9760	510.2402	0.01324	0.01627	0.02012	0.02219
TEMPO-P (core)	536.5199	571.9066	612.0213	631.9290	0.01824	0.02247	0.02784	0.03073
TEMPO-P	752.8377	808.4756	871.9199	903.5141	0.02812	0.03477	0.04325	0.04784
<b>12</b>	512.7627	543.0901	577.1995	594.0351	0.01628	0.01991	0.02447	0.02691
<b>12</b> -P (core)	608.6456	648.9624	694.4237	716.8988	0.02135	0.02617	0.03225	0.03551
<b>12</b> -P	822.3329	882.8646	951.6222	985.7696	0.03119	0.03842	0.04761	0.05257
<b>12</b> <sup>-</sup>	519.5040	549.2125	582.6009	599.0734	0.01611	0.01966	0.02412	0.02652
<b>12</b> <sup>-</sup> -P (core)	610.2006	649.9485	694.7405	716.8761	0.02118	0.02594	0.03193	0.03514
<b>12</b> <sup>-</sup> -P	828.0734	888.0477	956.1471	989.9598	0.03106	0.03822	0.04733	0.05224
<b>18</b> (core)	406.6822	424.3742	443.8138	453.2463	0.01071	0.01283	0.01543	0.01680
<b>18</b>	578.1478	614.9377	655.9061	675.9825	0.02001	0.02441	0.02989	0.03281
<b>18</b> -P (core)	507.7642	535.5589	566.4443	581.5525	0.01588	0.01921	0.02334	0.02554
<b>18</b> -P	860.3208	927.3224	1002.9629	1040.3668	0.03461	0.04262	0.05274	0.05817
<b>18</b> <sup>-</sup> (core)	396.1926	412.9170	431.2835	440.1921	0.01016	0.01216	0.01462	0.01591
<b>18</b> <sup>-</sup>	561.1984	596.9950	636.8692	656.4143	0.01935	0.02363	0.02897	0.03181
<b>18</b> <sup>-</sup> -P (core)	489.4501	516.1809	545.9089	560.4591	0.01515	0.01835	0.02233	0.02444
<b>18</b> <sup>-</sup> -P	861.6955	927.5023	1001.8670	1038.6638	0.03392	0.04179	0.05173	0.05707
<b>18</b> <sup>2-</sup> (core)	401.3742	417.3048	434.7592	443.2137	0.01003	0.01194	0.01428	0.01551
<b>18</b> <sup>2-</sup>	563.8712	598.9519	638.0153	657.1594	0.01918	0.02337	0.02860	0.03138

<b>18<sup>2-</sup>-P</b> (core)	486.6464	512.5596	541.3838	555.4930	0.01477	0.01787	0.02172	0.02377
<b>18<sup>2-</sup>-P</b>	843.8323	908.9928	982.6108	1019.0337	0.03363	0.04142	0.05127	0.05655
<b>7</b> (core)	482.0306	505.6145	505.6145	545.0549	0.01349	0.01631	0.01631	0.02174
<b>7</b>	631.3488	671.2195	671.2195	738.1197	0.02165	0.02642	0.02642	0.03562
<b>7-P</b> (core)	591.8265	625.4691	625.4691	681.9453	0.01881	0.02283	0.02283	0.03060
<b>7-P</b>	916.6096	986.7553	986.7553	1105.7134	0.03640	0.04478	0.04478	0.06114
<b>7<sup>-</sup></b> (core)	481.4011	504.3972	504.3972	542.7783	0.01337	0.01612	0.01612	0.02140
<b>7<sup>-</sup></b>	624.6312	663.8373	663.8373	729.5824	0.02137	0.02606	0.02606	0.03510
<b>7<sup>-</sup>-P</b> (core)	590.8048	623.8174	623.8174	679.1850	0.01862	0.02257	0.02257	0.03018
<b>7<sup>-</sup>-P</b>	910.4251	979.9047	979.9047	1097.7064	0.03612	0.04442	0.04442	0.06062
<b>17</b> (core)	407.9019	424.1683	442.2211	451.0548	0.01022	0.01217	0.01459	0.01587
<b>17</b>	627.7318	667.2289	711.7199	733.6974	0.02132	0.02604	0.03199	0.03518
<b>17-P</b> (core)	512.8174	538.9587	568.2517	582.6760	0.01519	0.01832	0.02224	0.02433
<b>17-P</b>	918.4367	988.1278	1067.2563	1106.5411	0.03619	0.04452	0.05510	0.06080
<b>17<sup>-</sup></b> (core)	402.5166	417.9926	435.1534	443.5465	0.00977	0.01162	0.01391	0.01513
<b>17<sup>-</sup></b>	627.1999	665.9738	709.6214	731.1756	0.02118	0.02581	0.03165	0.03478
<b>17<sup>-</sup>-P</b> (core)	498.7183	524.1651	552.6486	566.6659	0.01479	0.01783	0.02165	0.02368
<b>17<sup>-</sup>-P</b>	922.5335	991.6258	1070.0489	1108.9762	0.03606	0.04432	0.05480	0.06045
<b>14</b> (core)	406.8687	423.3917	441.9554	451.1128	0.00996	0.01193	0.01442	0.01575
<b>14</b>	593.7657	631.7264	674.4818	695.6142	0.02055	0.02509	0.03081	0.03388
<b>14-P</b> (core)	507.0254	533.3644	563.1166	577.8437	0.01484	0.01799	0.02197	0.02411
<b>14-P</b>	901.0274	969.2741	1046.7467	1085.2185	0.03552	0.04367	0.05403	0.05962
<b>14<sup>-</sup></b> (core)	406.2508	422.1011	439.8951	448.6688	0.00964	0.01154	0.01392	0.01519
<b>14<sup>-</sup></b>	587.3205	624.6007	666.5736	687.3151	0.02025	0.02471	0.03032	0.03333
<b>14<sup>-</sup>-P</b> (core)	507.8612	533.5877	562.6253	576.9920	0.01466	0.01773	0.02162	0.02370
<b>14<sup>-</sup>-P</b>	880.9000	948.4653	1025.1523	1063.2307	0.03509	0.04316	0.05342	0.05894
<b>15</b> (core)	449.2883	470.9900	495.3865	507.4145	0.01218	0.01478	0.01804	0.01979
<b>15</b>	562.0077	595.4004	632.8149	651.2262	0.01822	0.02221	0.02722	0.02989
<b>15-P</b> (core)	548.2920	579.9149	615.5913	633.2263	0.01720	0.02098	0.02576	0.02832
<b>15-P</b>	863.1363	926.7398	998.8100	1034.5375	0.03306	0.04066	0.05030	0.05548
<b>15<sup>-</sup></b> (core)	453.3353	474.4295	498.1050	509.7662	0.01209	0.01462	0.01778	0.01948
<b>15<sup>-</sup></b>	555.7988	588.5556	625.2242	643.2589	0.01800	0.02192	0.02683	0.02945
<b>15<sup>-</sup>-P</b> (core)	547.7785	578.7865	613.7398	631.0087	0.01703	0.02074	0.02542	0.02792
<b>15<sup>-</sup>-P</b>	865.5249	928.5087	999.8533	1035.2142	0.03289	0.04041	0.04995	0.05509
<b>13</b> (core)	561.8341	594.9018	631.7748	649.8634	0.01858	0.02253	0.02747	0.03009
<b>13</b>	479.7271	501.1403	525.0110	536.7175	0.01296	0.01552	0.01871	0.02042
<b>13<sup>-</sup></b> (core)	560.1305	592.5059	628.5806	646.2700	0.01824	0.02211	0.02694	0.02951
<b>13<sup>-</sup></b>	461.0339	481.8262	504.9697	516.3085	0.01252	0.01501	0.01811	0.01976
<b>13<sup>2-</sup></b> (core)	550.0501	581.6524	616.8664	634.1347	0.01783	0.02161	0.02632	0.02883
<b>13<sup>2-</sup></b>	472.9326	492.9664	515.2507	526.1656	0.01247	0.01486	0.01785	0.01943
<b>13-P</b> (core)	878.5915	941.8004	1013.2645	1048.6412	0.03339	0.04095	0.05051	0.05564
<b>13-P</b>	574.4855	605.6496	640.6582	657.9159	0.01768	0.02141	0.02609	0.02860
<b>13<sup>-</sup>-P</b> (core)	881.4979	944.1058	1014.8657	1049.8866	0.03317	0.04065	0.05011	0.05520
<b>13<sup>-</sup>-P</b>	577.0589	607.8670	642.3747	659.3553	0.01783	0.02151	0.02613	0.02860
<b>13<sup>2-</sup>-P</b> (core)	850.4836	912.2016	982.0023	1016.5629	0.03247	0.03985	0.04919	0.05420
<b>13<sup>2-</sup>-P</b>	566.8366	596.7388	630.2819	646.8029	0.01728	0.02085	0.02534	0.02774
<b>16</b> (core)	429.107	448.128	469.560	480.154	0.01113	0.01340	0.01627	0.01781
<b>16</b>	505.712	533.578	564.872	580.301	0.01542	0.01875	0.02294	0.02518
<b>16-P</b> (core)	542.155	571.111	603.816	620.006	0.01645	0.01991	0.02428	0.02663
<b>16-P</b>	815.659	873.622	939.462	972.160	0.03026	0.03718	0.04599	0.05073
<b>16<sup>-</sup></b> (core)	425.568	443.963	464.672	474.903	0.01088	0.01308	0.01585	0.01733
<b>16<sup>-</sup></b>	503.052	530.286	560.847	575.909	0.01517	0.01842	0.02251	0.02470
<b>16<sup>-</sup>-P</b> (core)	535.633	564.006	596.026	611.869	0.01618	0.01957	0.02386	0.02616

<b>16</b> <sup>-</sup> -P	808.513	865.852	930.969	963.303	0.02997	0.03682	0.04553	0.05022
<b>19</b> (core)	527.799	553.957	583.322	597.792	0.01505	0.01818	0.02210	0.02420
<b>19</b>	672.548	714.951	762.649	786.191	0.02313	0.02820	0.03458	0.03800
<b>19</b> -P (core)	634.542	670.748	711.490	731.602	0.02034	0.02467	0.03012	0.03304
<b>19</b> -P	959.784	1032.468	1114.886	1155.772	0.03790	0.04658	0.05761	0.06354
<b>19</b> <sup>-</sup> (core)	523.463	549.013	577.670	591.782	0.01483	0.01788	0.02172	0.02377
<b>19</b> <sup>-</sup>	668.006	709.778	756.746	779.923	0.02286	0.02786	0.03414	0.03750
<b>19</b> <sup>-</sup> -P (core)	626.828	662.342	702.310	722.040	0.01999	0.02423	0.02958	0.03244
<b>19</b> <sup>-</sup> -P	930.680	1002.624	1084.213	1124.690	0.03730	0.04589	0.05680	0.06268
<b>20</b> (core)	480.848	504.407	530.811	543.807	0.01346	0.01627	0.01981	0.02169
<b>20</b>	630.923	670.780	715.569	737.659	0.02164	0.02640	0.03239	0.03560
<b>20</b> -P (core)	589.591	623.227	661.044	679.698	0.01876	0.02278	0.02784	0.03055
<b>20</b> -P	927.939	998.001	1077.439	1116.843	0.03641	0.04479	0.05541	0.06113
<b>20</b> <sup>-</sup> (core)	478.645	501.602	527.297	539.932	0.01329	0.01604	0.01948	0.02131
<b>20</b> <sup>-</sup>	624.325	663.518	707.536	729.241	0.02137	0.02606	0.03195	0.03510
<b>20</b> <sup>-</sup> -P (core)	582.678	615.612	652.633	670.893	0.01843	0.02237	0.02733	0.02998
<b>20</b> <sup>-</sup> -P	911.675	981.082	1059.767	1098.794	0.03606	0.04436	0.05488	0.06054
<b>21</b> (core)	532.833	558.917	588.212	602.652	0.01505	0.01817	0.02209	0.02419
<b>21</b>	677.943	720.304	767.961	791.486	0.02318	0.02824	0.03462	0.03803
<b>21</b> -P (core)	629.106	665.250	705.942	726.034	0.02021	0.02453	0.02997	0.03289
<b>21</b> -P	972.029	1044.714	1127.138	1168.028	0.03800	0.04669	0.05771	0.06365
<b>21</b> <sup>-</sup> (core)	510.669	536.239	564.923	579.051	0.01468	0.01773	0.02157	0.02362
<b>21</b> <sup>-</sup>	650.646	692.428	739.408	762.590	0.02270	0.02770	0.03398	0.03735
<b>21</b> <sup>-</sup> -P (core)	625.967	661.475	701.439	721.167	0.01993	0.02418	0.02952	0.03239
<b>21</b> <sup>-</sup> -P	936.169	1008.037	1089.552	1129.996	0.03731	0.04590	0.05680	0.06267
<b>22</b> (core)	499.039	524.096	552.145	565.934	0.01426	0.01726	0.02101	0.02302
<b>22</b>	651.489	692.841	739.268	762.148	0.02244	0.02738	0.03360	0.03692
<b>22</b> -P (core)	608.081	643.211	682.666	702.110	0.01958	0.02378	0.02906	0.03188
<b>22</b> -P	942.704	1014.231	1095.278	1135.457	0.03716	0.04571	0.05655	0.06238
<b>22</b> <sup>-</sup> (core)	551.870	580.768	612.906	628.630	0.01670	0.02015	0.02446	0.02674
<b>22</b> <sup>-</sup>	691.520	736.629	787.071	811.857	0.02468	0.03007	0.03682	0.04042
<b>22</b> <sup>-</sup> -P (core)	651.345	690.182	733.612	754.946	0.02176	0.02641	0.03222	0.03532
<b>22</b> <sup>-</sup> -P	987.844	1063.171	1148.276	1190.381	0.03947	0.04847	0.05986	0.06597
<b>23</b> (core)	535.131	562.749	593.742	609.004	0.01566	0.01896	0.02311	0.02533
<b>23</b>	682.238	726.120	775.462	799.804	0.02376	0.02901	0.03561	0.03915
<b>23</b> -P (core)	638.904	676.503	718.820	739.704	0.02083	0.02532	0.03098	0.03402
<b>23</b> -P	977.049	1051.124	1135.105	1176.754	0.03853	0.04739	0.05862	0.06466
<b>23</b> <sup>-</sup> (core)	573.702	605.294	640.521	657.786	0.01797	0.02174	0.02646	0.02897
<b>23</b> <sup>-</sup>	715.218	763.016	816.541	842.865	0.02594	0.03166	0.03882	0.04265
<b>23</b> <sup>-</sup> -P (core)	674.030	715.558	762.073	784.946	0.02304	0.02801	0.03423	0.03756
<b>23</b> <sup>-</sup> -P	994.776	1072.763	1160.916	1204.541	0.04063	0.04995	0.06174	0.06807

<sup>a</sup> P• = •CH(Ph)CH<sub>2</sub>CH(Ph)CH<sub>3</sub> dimeric propagating styryl radical, see main text for the structures of the nitroxide radicals.

## Optimised geometries

NOTE: All species had zero imaginary frequencies, as determined from frequency calculations at the M06-2X/6-31+G(d) level.

```
P• (core) 1\1\GINC-X150\FOpt\UM062X\Gen\C4H7(2)\GXG501\05-Dec-2012\0\#M062X/gen
6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=536870912\b
ps_rcore1.freq\b\0,2\c,-6.25570113,2.5656944662,0.3319762147\h,-5.45497
10416,1.8482181447,0.506927101\c,-6.0111013036,3.6255896513,-0.5280886
555\c,-7.5516957595,2.3398192122,1.0394983559\h,-7.9892402474,1.368682
3453,0.7744785349\h,-7.418432169,2.3358602604,2.1289767048\h,-8.279921
0265,3.1177563144,0.7908089298\h,-6.8238807103,4.3345726668,-0.6918953
89\c,-4.8161701938,3.847174945,-1.1899532913\h,-3.9742024037,3.1732759
514,-1.0636491403\h,-4.6836267187,4.6948672305,-1.8512362283\b\Version=
EM64L-G09RevB.01\b\State=2-A\HF=-156.4900274\b\S2=0.781102\b\S2-1=0.\b\S2A=0.7
50209\b\RMSD=8.591e-09\b\RMSF=6.199e-06\b\Di pole=-0.1383044,-0.1045496,0.133
1834\b\Quadrupole=0.5977329,0.2591743,-0.8569073,-0.6591418,-0.7214828,-
1.5012305\b\PG=C01 [X(C4H7)]\@\b

P•
1\1\GINC-X109\FOpt\UM062X\Gen\C16H17(2)\GXG501\04-Jun-2012\0\#M062X/g
en
6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280
\b\dps_r.freq\b\0,2\c,-6.3184623736,2.4937462438,0.2225996346\c,-5.34235
98299,1.3184769407,0.0964984526\c,-4.1180921579,1.7204895037,-0.741715
1227\c,-3.143848822,0.60561344,-0.9432939502\h,-7.2056862086,2.2062847
314,0.7946664598\h,-6.6401551863,2.8399160108,-0.7657175353\h,-5.84552
70942,3.3369075248,0.7391989311\h,-5.8531466817,0.5054389367,-0.437925
9347\c,-4.9498674785,0.7860161308,1.4622587037\h,-3.6196419415,2.58119
43821,-0.2638726283\h,-4.4712161642,2.0972865518,-1.7147263624\h,-3.32
66507488,-0.3332364779,-0.4252464254\c,-1.9823322363,0.7029370854,-1.7
539288398\c,-4.1838929109,1.5581840842,2.343801552\c,-3.8352563159,1.0
733574927,3.6014654846\c,-4.2479646589,-0.1975810277,4.0030115695\c,-5
.0104612803,-0.9760259615,3.1362394623\c,-5.355836195,-0.4845955899,1.
8767617458\c,-1.1115815398,-0.409014064,-1.8955305041\c,0.0253961052,-
0.3351941376,-2.6826207857\c,0.3419004147,0.8485486503,-3.3593338373\c
,-0.4991567459,1.9573962132,-3.2333756413\c,-1.6408516455,1.8927387288
,-2.4470318809\h,-3.8511310745,2.549950936,2.044544458\h,-3.237811444,
1.6873043456,4.2695035938\h,-3.9747249847,-0.5766868886,4.9833224204\h
,-5.3363757513,-1.9677854619,3.4368928929\h,-5.9502026229,-1.098550945
9,1.2029744333\h,-1.3522042737,-1.330412069,-1.3704241231\h,0.67437290
04,-1.2016618918,-2.7736238778\h,1.2336754118,0.9051521797,-3.97589858
79\h,-0.2587969469,2.8801110555,-3.7542655517\h,-2.2809695179,2.766173
3482,-2.3598812056\b\Version=EM64L-G09RevB.01\b\State=2-A\HF=-619.6364285
\b\S2=0.773921\b\S2-1=0.\b\S2A=0.750349\b\RMSD=4.427e-09\b\RMSF=5.385e-06\b\Di pole
=-0.2054509,0.0682104,0.0782799\b\Quadrupole=-1.4857546,2.9229656,-1.437
2109,0.5570573,-0.0093783,-2.4124882\b\PG=C01 [X(C16H17)]\@\b

TEMPO
1\1\GINC-X93\FOpt\UM062X\Gen\C9H18N1O1(2)\GXG501\07-May-2012\0\#M062X
/gen
6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=13421772
80\b\jtempo_r.freq\b\0,2\N,0.,-0.7354390395,-0.2577501566\O,0.,-2.006628
9532,-0.1603088566\c,0.,2.1196766418,0.020768313\h,0.,3.1551331371,-0.
3367835653\h,0.,2.1697471177,1.1166915241\c,1.2418324841,1.3946082342,
-0.4878446086\c,-1.2418324841,1.3946082342,-0.4878446086\c,1.316800953
,-0.0700401012,-0.03759592\c,-1.316800953,-0.0700401012,-0.03759592\c,
2.3481811493,-0.814606545,-0.8874814602\c,-2.3481811493,-0.814606545,-
0.8874814602\c,1.7056923723,-0.1864514354,1.4445454599\c,-1.7056923723
,-0.1864514354,1.4445454599\h,2.1583734633,1.8970132594,-0.1555401175\
h,-2.1583734633,1.8970132594,-0.1555401175\h,1.2409515557,1.4240794878
,-1.5863987363\h,-1.2409515557,1.4240794878,-1.5863987363\h,2.02865056
24,-0.8473336243,-1.9338349492\h,-2.0286505624,-0.8473336243,-1.933834
9492\h,3.3077389221,-0.289828342,-0.8290734391\h,-3.3077389221,-0.2898
28342,-0.8290734391\h,2.4794085877,-1.8392995501,-0.5349634993\h,-2.47
94085877,-1.8392995501,-0.5349634993\h,2.7521011046,0.1111332219,1.572
9166315\h,-2.7521011046,0.1111332219,1.5729166315\h,1.093576775,0.4498
067943,2.0894625254\h,-1.093576775,0.4498067943,2.0894625254\h,1.59514
82111,-1.2248497809,1.7709006526\h,-1.5951482111,-1.2248497809,1.77090
06526\b\Version=EM64L-G09RevB.01\b\State=2-A'\HF=-483.5045887\b\S2=0.754857
\b\S2-1=0.\b\S2A=0.750014\b\RMSD=6.749e-09\b\RMSF=7.711e-06\b\Di pole=0.,1.237629
```

5,0.1376479\Quadrupole=3.0887821,-3.8750089,0.7862268,0.,0.,-0.7405013  
\PG=CS [SG(C1H2N1O1),X(C8H16)]\\@

TEMPO-P (core)

```
1\1\GINC-X146\FOpt\RM062X\Gen\C13H25N1O1\GXG501\05-Dec-2012\0\#\M062X/
gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=536870912
\dst_core1.freq\0,1\N,-1.9304325296,-0.3571821999,-0.1017369309\O,-1
.0998789908,0.066406383,0.9752783749\C,-1.0811635314,-0.4270900696,-1
.3257163823\C,-3.1161026571,0.5508899817,-0.1357518171\C,-1.1586573343,
-0.8073632292,2.1114014196\H,-2.1743025856,-1.2042246175,2.2020458474\
C,-0.8181907201,0.0763533998,3.3063940438\C,-0.1984294017,-1.960803438
3,2.0187598279\H,0.1889970494,0.4908798847,3.1914322754\H,-1.524054320
5,0.909408372,3.3797649552\H,-0.8505617718,-0.5057495688,4.2316255759\
H,0.8515137239,-1.6954244414,1.8869171019\C,-0.5612953968,-3.235092423
8,2.1462416539\H,-1.606191399,-3.5112876987,2.2728376777\H,0.163385199
,-4.0437646906,2.1213578707\C,-0.2847403359,0.8552052198,-1.6364058738
\C,-0.0749369236,-1.5644170401,-1.1333632726\C,-2.7812578756,2.0539959
639,-0.1720307671\C,-3.9435234668,0.2927048991,1.1297190286\C,-3.97652
13282,0.1426479819,-1.3424246042\C,-1.9971377973,-0.8072485045,-2.5002
442004\C,-3.199230187,0.1172924261,-2.6528946139\H,0.6958577956,-1.291
690923,-0.4079713623\H,0.4192861142,-1.7747279443,-2.0886535844\H,-0.5
778310778,-2.4702064522,-0.7845937612\H,0.1515078997,1.2621698304,-0.7
198480211\H,0.5334710003,0.6095877551,-2.322556158\H,-0.8840941186,1.6
329785063,-2.1127579506\H,-1.9711686686,2.2772705854,0.5281964981\H,-2
.4926525561,2.4073235359,-1.1632163778\H,-3.6639677168,2.6270367575,0.
1329970241\H,-4.8995142251,0.8218779571,1.0510597811\H,-3.4342437519,0
.6613551233,2.0258277073\H,-4.1498891324,-0.7759266012,1.2464339256\H,
-4.8280967763,0.8320874717,-1.4010232448\H,-4.382681771,-0.8601491415,
-1.1511766158\H,-1.3895198106,-0.8165159233,-3.4136603142\H,-2.3549738
558,-1.8332037693,-2.3375087157\H,-2.877365639,1.1282587385,-2.9311932
993\H,-3.844396129,-0.2355880958,-3.4654237216\Version=EM64L-G09RevB.
01\State=1-A\HF=-640.0577421\RMSD=7.691e-09\RMSF=6.729e-06\Dipole=-0.1
999216,-0.0569044,-0.0672851\Quadrupole=0.3867714,-1.056975,0.6693261
,-1.0309484,0.2470134,-0.559198\PG=C01 [X(C13H25N1O1)]\\@
```

TEMPO-P

```
1\1\GINC-X147\FOpt\RM062X\Gen\C25H35N1O1\GXG501\16-Jun-2012\0\#\M062X/
gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=134217728
0\dst.freq\0,1\N,1.0981174835,-0.0562329823,-0.257391388\O,0.1756579
892,0.6070226181,0.6069557603\C,-0.8911686754,1.2452144287,-0.10816093
31\C,3.6256551451,-1.3809721894,-0.7174309202\H,4.3167003646,-1.885622
3453,-1.402175843\H,4.1170661834,-1.3680855713,0.2631977776\C,-1.26506
8341,2.4743826425,0.7213915949\C,-2.0755411567,0.3301512016,-0.3415432
329\C,1.6052608548,-1.5850135593,1.7252460608\C,2.9316588532,1.1807051
576,1.0253060724\C,1.2491418468,-1.4571010944,0.2317075091\C,2.3281208
459,0.7881316386,-0.3363784641\C,-0.0799026368,-2.183502966,0.00626613
13\C,1.9679539851,2.083931625,-1.0749889811\C,2.3073005489,-2.14175940
25,-0.6492276299\C,3.3528961376,0.0373570662,-1.2020571151\H,1.8976959
498,-2.2366371632,-1.6643352943\H,2.9674186554,-0.0068931688,-2.229985
8164\H,2.458511794,-3.1580608888,-0.2648637217\H,4.2748884748,0.631709
9175,-1.2268564473\H,0.0717153152,-3.2605780497,0.141103935\H,2.885784
3121,2.6402228547,-1.2961957203\H,-0.4528213515,-2.0038156777,-1.00658
13136\H,1.4581861945,1.8710875612,-2.0201497542\H,-0.8406129611,-1.856
7452068,0.7183187046\H,1.3287148292,2.7312841191,-0.4674623527\H,1.385
476067,-2.6057042675,2.0577260077\H,3.6026547966,2.0362240599,0.888923
2696\H,2.6583811086,-1.3934264038,1.9383048457\H,3.5151919035,0.380849
3972,1.4842001821\H,0.9977785191,-0.8965110098,2.319495423\H,2.1388960
592,1.475925433,1.7187167045\H,-0.3581986209,3.0750632866,0.8709840863
\C,-2.3647905455,3.3386241363,0.0843884238\H,-1.5898394401,2.152719330
5,1.7194025984\H,-0.5129222651,1.562362268,-1.0837352992\C,-2.45093081
61,-0.0119554144,-1.6404708492\C,-3.5389454486,-0.855689744,-1.8701583
634\C,-4.2634412176,-1.3647122081,-0.7950884792\C,-3.8978673409,-1.024
0523921,0.5090936868\C,-2.8140778047,-0.179753111,0.7313171347\H,-1.87
92732838,0.3829125994,-2.4779745627\H,-3.8158090052,-1.1181683204,-2.8
87429216\H,-5.1087286866,-2.0243309658,-0.9691767679\H,-4.4574215115,-
1.4208128747,1.3516037273\H,-2.5207418299,0.0659343727,1.7499401159\H,
-3.2746704806,2.7281206192,0.0129010917\C,-1.9912854687,3.7632330186,-
1.324180726\C,-2.6728587578,4.5494462875,0.9730366884\C,-2.7736520834,
3.3821808737,-2.4173295685\C,-2.4208702245,3.7489944006,-3.7165318896\
C,-1.2728277988,4.5051063111,-3.9417137363\C,-0.4848548035,4.896197851
5,-2.8586019587\C,-0.8442648219,4.5296918053,-1.5640516293\H,-3.663527
9723,2.7794821147,-2.2473088732\H,-3.0432459692,3.4406571838,-4.552087
```

7742\H,-0.9933002133,4.7894888064,-4.9519566662\H,0.4120941485,5.48699  
 52712,-3.0229230975\H,-0.2188101249,4.8411098849,-0.7293701528\H,-2.98  
 74522931,4.2254909906,1.9710435224\H,-3.4710913469,5.1595525239,0.5394  
 40785\H,-1.7884064921,5.1860634323,1.0893208348\\Version=EM64L-G09RevB  
 .01\State=1-A\HF=-1103.2139093\RMSD=6.098e-09\RMSF=2.069e-06\Dipole=0.  
 0534768,-0.0308389,-0.1550527\Quadrupole=2.3038589,-3.2945203,0.990661  
 5,3.843377,-0.987364,0.1617162\PG=C01 [X(C25H35N1O1)]\\@

**12**

1\\1\GINC-X156\FOpt\UM062X\6-31+G(d)\C10H18N1O3(2)\GXG501\10-Aug-2012\0  
 \\#M062X/6-31+G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) ma  
 xdisk=1342177280\\pipoh\_r+.freq\\0,2\N,1.5434534514,-0.2847625396,0.03  
 58220029\O,2.8179792757,-0.2893900232,0.0354623211\C,-1.2728625476,0.2  
 353959538,0.0318345672\C,-2.7477319799,-0.0954997492,0.0215422194\H,-1  
 .2010915304,1.3303909034,-0.0064052843\C,-0.5962570448,-0.3593266476,-  
 1.2100126653\C,-0.5985377873,-0.320529401,1.2787660518\C,0.8998854018,  
 -0.0315269737,-1.2844471506\C,0.8964346366,0.0095400646,1.3470793486\C  
 ,1.5660262233,-0.9613014455,-2.3008527332\C,1.5626916116,-0.8876723188  
 ,2.3920455999\C,1.1391064398,1.4276485034,-1.7018104017\C,1.1388168104  
 ,1.4810276528,1.7183239382\H,-1.0757023609,0.004910148,-2.1249369846\H  
 ,-1.0818292231,0.0611070035,2.1850796591\H,-0.72257541,-1.4504877185,-  
 1.1822474636\H,-0.7340248451,-1.409313443,1.2872451649\H,1.5084167799,  
 -2.0007056145,-1.9632242554\H,1.5043926191,-1.9370945321,2.0872960364\  
 H,1.0499744177,-0.8735230584,-3.2626892352\H,1.0445832486,-0.770568391  
 7,3.3495171515\H,2.6172291021,-0.6997987338,-2.4341417904\H,2.61378136  
 87,-0.6223278553,2.5189206207\H,0.8479789096,1.5623078693,-2.748946031  
 8\H,0.84382301,1.6489872304,2.7595862818\H,0.5663085421,2.1384354387,-  
 1.0998790222\H,0.5697132402,2.173831721,1.0921648373\H,2.2023927251,1.  
 6639727694,-1.6006321826\H,2.2029755483,1.7124535953,1.6145560428\O,-3  
 .3174035172,-0.817639521,0.8021829314\O,-3.3882742014,0.5103813745,-1.  
 0012997527\H,-4.323159848,0.2425304743,-0.9580912233\\Version=EM64L-G0  
 9RevB.01\State=2-A\HF=-672.0181603\S2=0.754852\S2-1=0.\S2A=0.750014\RM  
 SD=4.307e-09\RMSF=1.433e-05\Dipole=-0.820088,0.5707814,-0.4492155\Quad  
 rupole=-5.1004406,1.1184692,3.9819714,-1.227641,3.966383,1.9381343\PG=  
 C01 [X(C10H18N1O3)]\\@

**12-P (core)**

1\\1\GINC-X139\FOpt\RM062X\Gen\C14H25N1O3\GXG501\06-Dec-2012\0\\#M062X/  
 gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=536870912  
 \\dstc\_core1.freq\\0,1\N,-1.3031444351,0.091746048,0.3592668604\O,-0.2  
 218790071,0.4557603579,1.2095997157\C,1.0556471393,0.3954805716,0.5567  
 98173\C,-4.074169753,-0.5970782223,-0.0432043798\C,-5.2220404798,-0.96  
 82406876,-0.9520417386\H,-4.4945389723,-0.5225202812,0.9680049146\C,2.  
 0573428377,0.131584719,1.6752488907\C,1.4023875559,1.6621966788,-0.175  
 064833\C,-2.7560525933,1.5999148397,1.8263378481\C,-2.0724220863,-1.42  
 99770604,2.2668545628\C,-2.3058752195,1.1927233822,0.4098825215\C,-1.7  
 562605299,-1.2714780135,0.7673903829\C,-1.6850754814,2.4251483185,-0.2  
 533992169\C,-0.635806891,-2.2619061473,0.4257913785\C,-3.5046560068,0.  
 7670388413,-0.4513500353\C,-2.9663134664,-1.6380307426,-0.1034024873\H  
 ,-3.179928628,0.7111226267,-1.4994061641\H,-2.6419496636,-1.739053545,  
 -1.1463229957\H,-4.2759318399,1.541772317,-0.3809816077\H,-3.339969858  
 5,-2.6198712472,0.2098348642\H,-2.4622191209,3.180369756,-0.4156152626  
 \H,-1.0032451189,-3.2848985612,0.5596574555\H,-1.2352981505,2.16171615  
 9,-1.2141047971\H,-0.3180369866,-2.1438622966,-0.6147356467\H,-0.91395  
 51273,2.8657235145,0.3834132604\H,0.2282328707,-2.1310845073,1.0847033  
 247\H,-3.2122546989,2.5949402328,1.7844395815\H,-2.0757188091,-2.49504  
 57918,2.5230559181\H,-3.4942339118,0.9244001019,2.2622235767\H,-3.0457  
 349609,-1.026679931,2.5513383265\H,-1.892605081,1.6490503798,2.4954842  
 243\H,-1.3031581371,-0.93685476,2.8678887059\H,1.8102460835,-0.7963898  
 891,2.1999837608\H,3.0696579966,0.0563225974,1.268551996\H,2.034479846  
 6,0.9515104989,2.4009428125\H,1.0488273134,-0.4319851232,-0.1588476944  
 \C,1.7437856446,1.7010261673,-1.4610275493\H,2.0352934535,2.6261126791  
 ,-1.9498156611\H,1.4106850947,2.5720048204,0.427023464\O,-6.2759412422  
 ,-0.1373473118,-0.7919974641\O,-5.23578237,-1.8749881935,-1.7485361028  
 \H,-6.9651769815,-0.4220544723,-1.4174629157\H,1.7352607721,0.80052317  
 7,-2.0718479672\\Version=EM64L-G09RevB.01\State=1-A\HF=-828.572222\RM  
 SD=5.941e-09\RMSF=2.792e-06\Dipole=0.0893002,0.3988175,0.2829242\Quad  
 rupole=4.6846197,-1.8370483,-2.8475713,-2.6808187,-1.1363689,-4.1679434  
 \PG=C01 [X(C14H25N1O3)]\\@

**12-P**

1\\1\GINC-X152\FOpt\RM062X\Gen\C26H35N1O3\GXG501\22-Jun-2012\0\\#M062X/  
 gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=134217728

```

0\\dsc.freq\\0,1\\N,-1.8901567036,-0.3579420938,-0.1547864285\\O,-1.085
2561557,0.0830518717,0.936437536\\C,0.2821347105,0.3045194616,0.559542
1176\\C,-4.3394705585,-1.4745447042,-1.1924586239\\C,-5.199469456,-1.924
5233201,-2.3494700023\\H,-4.9468977047,-1.6056789942,-0.2876943681\\C,1.
1088804388,-0.0185025676,1.8043265426\\C,0.5328983977,1.7083902622,0.04
97853061\\C,-3.8668628626,0.6708865091,1.0964880337\\C,-2.681116714,-2.2
293559757,1.3982253071\\C,-3.0833442032,0.5318313581,-0.2229419169\\C,-2
.1269524735,-1.8224748865,0.01963717\\C,-2.6124017878,1.9301066455,-0.6
342261918\\C,-0.7878752607,-2.5468779689,-0.1722364103\\C,-3.9875066827,
0.0094031708,-1.350035965\\C,-3.0535703025,-2.2829033947,-1.1148302826\\
H,-3.4661487807,0.1452929022,-2.3075324534\\H,-2.5256557952,-2.18802148
39,-2.071596089\\H,-4.8969637616,0.6195129386,-1.3751634787\\H,-3.272731
2525,-3.3481895272,-0.9772172405\\H,-3.4818698325,2.5370538881,-0.91076
72441\\H,-0.9650545275,-3.6269451778,-0.2195060805\\H,-1.9325735349,1.87
49923277,-1.4895555097\\H,-0.3007424926,-2.2376714045,-1.1023715462\\H,-
2.0958707914,2.4316539233,0.1865545113\\H,-0.1063444378,-2.3602648571,0
.6628319382\\H,-4.5040562228,1.5602377508,1.0415386524\\H,-2.5196874974,
-3.3024026652,1.5488028386\\H,-4.5159191986,-0.1798118016,1.312611691\\H
,-3.7512181101,-2.0449576185,1.5083903533\\H,-3.1737421924,0.8000103884
,1.9324134036\\H,-2.1530719246,-1.6902035095,2.1899101424\\H,0.848835814
1,-1.0332516901,2.1336096402\\C,2.6258274594,0.0836642792,1.5784628062\\
H,0.816911316,0.6553967646,2.6200991145\\H,0.5371423504,-0.3947774781,-
0.2409586061\\C,0.9388479678,1.9116100829,-1.2691128291\\C,1.1691873192,
3.20005812,-1.754207444\\C,0.9946907873,4.2997889922,-0.9174619182\\C,0.
5933904121,4.1057869901,0.4061106791\\C,0.3687389223,2.8184443746,0.884
8631958\\H,1.0682137043,1.0506267748,-1.9219315374\\H,1.4793598411,3.343
3300022,-2.7855152034\\H,1.1698322623,5.304305554,-1.2918208826\\H,0.453
3907493,4.960189333,1.0623903416\\H,0.0371467548,2.6743688826,1.9111705
095\\H,2.8573741091,1.1220402893,1.306549729\\C,3.0728732151,-0.79838321
31,0.4269038636\\C,3.3810485325,-0.2493872749,2.8703729898\\C,3.66190555
44,-0.244139287,-0.712451176\\C,4.0474243284,-1.0482393768,-1.785701076
8\\C,3.8464973096,-2.4256648419,-1.7343470212\\C,3.264396339,-2.99284372
74,-0.6002314444\\C,2.8847919211,-2.185238079,0.4688969162\\H,3.80872250
59,0.8328910995,-0.7624715597\\H,4.5022453787,-0.5959650207,-2.66266674
37\\H,4.1415771351,-3.0540418196,-2.5695538812\\H,3.104506952,-4.0663052
445,-0.5492386969\\H,2.4308206895,-2.6423501633,1.3463045243\\H,3.083049
0274,0.4289901861,3.67714577\\H,4.4619106954,-0.1605030295,2.7249366251
\\H,3.1688381034,-1.2737794974,3.1969025652\\O,-6.4133903294,-1.33045766
18,-2.3316864081\\O,-4.8794370984,-2.7023415223,-3.2152737459\\H,-6.9013
013578,-1.6485332447,-3.1114238084\\Version=EM64L-G09RevB.01\\State=1-A
\\HF=-1291.7285633\\RMSD=9.802e-09\\RMSF=1.097e-05\\Dipole=0.0039372,0.456
4478,0.3230501\\Quadrupole=0.5296157,1.3399657,-1.8695815,-0.4707739,-2
.354429,-4.1110707\\PG=C01 [X(C26H35N1O3)]\\@
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12-

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1\\1\\GINC-V1310\\FOpt\\UM062X\\6-31+G(d)\\C10H17N1O3(1-,2)\\GXG501\\21-Feb-20
12\\0\\#M062X\\6-31+G(d) 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4
) Freq=noramman maxdisk=268435456\\\\piro_r.freq\\-1,2\\N,-0.1453667125,0.
2305387129,0.0538396144\\C,-0.0056807628,0.0079619128,1.5233372907\\C,1.
4740689119,-0.0106769564,1.9258320149\\C,2.2954571829,1.1146938993,1.31
55037378\\C,2.1985426804,1.0149098227,-0.2003917675\\C,0.7673267854,1.10
23512906,-0.7429439659\\C,3.7906218966,1.1077148692,1.8020422102\\O,4.00
54798471,0.5140600443,2.8826163845\\O,4.5876269097,1.7273944222,1.06134
30586\\C,0.7256137937,0.5966545852,-2.1869478553\\H,0.3794626455,3.00384
3155,0.2793693643\\C,-0.7784080934,1.1101464413,2.266058191\\C,-0.646998
8355,-1.3463119378,1.8356076867\\O,-1.3096404172,0.0377380939,-0.436500
0888\\C,0.2363793657,2.5443664629,-0.7022132284\\H,1.8946950236,2.087445
4833,1.6424454603\\H,1.9176723442,-0.9672581118,1.6138682733\\H,2.635633
7895,0.0535686729,-0.509904445\\H,1.5503486653,0.0183237584,3.017648250
5\\H,2.8096693146,1.7978274032,-0.6610321068\\H,-0.475850983,-1.58304520
56,2.8914458913\\H,1.4592341763,1.1555708781,-2.7781725476\\H,-0.1886518
301,-2.1312491486,1.2250733591\\H,0.9869212291,-0.4660868175,-2.2231784
784\\H,-1.7215067842,-1.3333907625,1.6361858312\\H,-0.2672969133,0.72558
29184,-2.6250778516\\H,-0.8503174179,0.8498037315,3.3281407021\\H,0.7776
942201,3.1509339724,-1.4369769199\\H,-0.2774587529,2.079116474,2.193013
6171\\H,-1.7886894883,1.1988753115,1.8527459232\\H,-0.8305262763,2.55455
12199,-0.9491649398\\Version=EM64L-G09RevB.01\\State=2-A\\HF=-671.475773
9\\S2=0.754988\\S2-1=0.\\S2A=0.750016\\RMSD=3.057e-09\\RMSF=1.948e-06\\Dipol
e=-3.9696434,-0.237245,-1.4237149\\Quadrupole=-25.3187181,16.7785121,8.
540206,-7.825027,-17.0622158,-0.263221\\PG=C01 [X(C10H17N1O3)]\\@
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**12<sup>-</sup>P (core)**

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1\1\GINC-X152\FOpt\RM062X\Gen\C14H24N1O3(1-)\GXG501\06-Dec-2012\0\\#M0
62X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=53687
0912\dstca_core1.freq\,-1,1\N,-1.3667349268,0.1095491245,0.3313059106
\O,-0.2888983726,0.4692042962,1.2045289115\C,0.988986346,0.3404811977,
0.5850727709\C,-4.1711865845,-0.5055209942,-0.1208502822\C,-5.39516775
46,-0.8718475774,-1.0332368237\H,-4.5946424583,-0.3907305658,0.8890078
527\C,1.9623771966,0.0493327113,1.724472315\C,1.4130427538,1.581363704
8,-0.1541646462\C,-2.795281771,1.718785848,1.703679279\C,-2.2198669138
,-1.3258066912,2.2633635794\C,-2.3381654283,1.2416621777,0.3110149928\
C,-1.8764803451,-1.2266556923,0.7643979487\C,-1.6570681299,2.424749606
2,-0.3832680835\C,-0.7799039203,-2.2611732754,0.4755545468\C,-3.539346
0502,0.8123998992,-0.5468992895\C,-3.092346528,-1.5758958811,-0.109691
963\H,-3.2019454809,0.7159564357,-1.58965232\H,-2.7531173144,-1.735202
1453,-1.1423690175\H,-4.2958433472,1.6041585532,-0.5300610829\H,-3.509
3437696,-2.5318353245,0.2260772307\H,-2.4095778508,3.1919134863,-0.598
7820162\H,-1.1904528473,-3.2658029712,0.6256484067\H,-1.1989137115,2.1
050506115,-1.3235012485\H,-0.4425677259,-2.1826012509,-0.5632543827\H,
-0.8843176853,2.8734360925,0.2495109702\H,0.0803560744,-2.1475413983,1
.1459967879\H,-3.2253618304,2.7227846775,1.6096318538\H,-2.271326251,-
2.3834101037,2.5478529863\H,-3.5650936485,1.0792168779,2.1379335639\H,
-3.1863347336,-0.8804797569,2.5032774314\H,-1.9460961975,1.7720595582,
2.3926729988\H,-1.4461696076,-0.8434475923,2.8697517969\H,1.6572131762
,-0.8552528892,2.2595656922\H,2.9778599965,-0.0822434065,1.338361706\H
,1.9644879972,0.8825477948,2.4360963052\H,0.9640356219,-0.49524336,-0.
121280652\C,1.8108734207,1.5895388599,-1.4245221362\H,2.1422893397,2.4
994777067,-1.9172762526\H,1.4140387767,2.5023015469,0.4311959018\H,1.7
921489333,0.6809541166,-2.0229767387\O,-5.4772593516,-2.0702086981,-1.
387027564\O,-6.1662850965,0.0842376911,-1.2810772399\Version=EM64L-G0
9RevB.01\State=1-A\HF=-828.0225077\RMSD=4.038e-09\RMSF=5.915e-06\Dipol
e=6.2071598,1.5000826,2.4296438\Quadrupole=-30.8420745,15.8387917,15.0
032828,-12.6262615,-23.0086511,-6.2593611\PG=C01 [X(C14H24N1O3)]\\@
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**12<sup>-</sup>P**

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1\1\GINC-X90\FOpt\RM062X\Gen\C26H34N1O3(1-)\GXG501\23-Jun-2012\0\\#M06
2X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=134217
7280\dstca.freq\,-1,1\N,-1.9255048181,-0.3931747804,-0.1267247174\O,-
1.1025319173,0.0812920589,0.9514059864\C,0.2529403172,0.2712401325,0.5
556382541\C,-4.4242629587,-1.5175387737,-1.1020401733\C,-5.388487085,-
2.0262111233,-2.2317243682\H,-5.0077443146,-1.6012365211,-0.1720161718
\C,1.0987442901,-0.0705519673,1.7859089916\C,0.5349684829,1.67803896,0
.0630763257\C,-3.8647133902,0.7394776289,1.0832977807\C,-2.7220668532,
-2.1834563041,1.5088833619\C,-3.1055311383,0.5131203271,-0.2383620331\
C,-2.1870603675,-1.8463405452,0.1040142131\C,-2.6046693529,1.876617205
2,-0.7257724643\C,-0.8595825486,-2.5960780812,-0.0770352236\C,-4.03832
7781,-0.0613440182,-1.3175296743\C,-3.1506429823,-2.3377700434,-0.9891
873707\H,-3.5336387124,0.0248645038,-2.2914413563\H,-2.6335903518,-2.3
084155741,-1.9580766538\H,-4.9426460277,0.553775978,-1.3740371687\H,-3
.390940504,-3.3903802491,-0.8028946694\H,-3.4649237821,2.4777056651,-1
.0417474397\H,-1.058634321,-3.6736167711,-0.0894242954\H,-1.9316380862
,1.7549952087,-1.5805572256\H,-0.3850777908,-2.3253548696,-1.026239622
1\H,-2.0765083086,2.4229247024,0.0606438672\H,-0.1597370961,-2.3959051
615,0.7419038628\H,-4.4950623975,1.6302880512,0.9793790505\H,-2.588752
2766,-3.2560947243,1.6929237053\H,-4.5222439668,-0.0920928886,1.341367
2759\H,-3.786157842,-1.9678463146,1.6150953169\H,-3.1642788082,0.90882
15496,1.9076993415\H,-2.17005623,-1.6309186226,2.2763751007\H,0.851385
8195,-1.094410743,2.0941317186\C,2.6135395449,0.0647962068,1.568481717
3\H,0.7973708942,0.580839486,2.6170686592\H,0.4830211283,-0.4249834946
,-0.2564466451\C,0.9910981936,1.8931805689,-1.23685458\C,1.2612395305,
3.1841477974,-1.6942169987\C,1.0773743107,4.2754674724,-0.8486334349\C
,0.6205081395,4.0698815309,0.4552450422\C,0.3543895448,2.7802869685,0.
9052145766\H,1.1215706504,1.0398047012,-1.8990588161\H,1.6041464028,3.
3359415718,-2.714194178\H,1.2794473234,5.2824563018,-1.2034868418\H,0.
462623177,4.9181242594,1.1161245419\H,-0.0303008176,2.6248266254,1.911
2143884\H,2.8323154628,1.1210758534,1.3624838759\C,3.0917147728,-0.735
8537871,0.3713134184\C,3.3718226877,-0.3386268262,2.839362508\C,3.7678
988224,-0.1128090181,-0.6806785535\C,4.1968201914,-0.8403847403,-1.791
2139261\C,3.9501226086,-2.2091993578,-1.8670797869\C,3.2773815892,-2.8
443500693,-0.8227305231\C,2.8577090634,-2.1135852349,0.285678564\H,3.9
396480085,0.9608613994,-0.6366089045\H,4.7132381086,-0.333394453,-2.60
19567451\H,4.2698541011,-2.7768027986,-2.7362930366\H,3.0677675057,-3.
9090068315,-0.8768647037\H,2.3230512614,-2.6208938169,1.0861447599\H,3
```

.0497949844,0.2716242999,3.6906520294\H,4.4515952741,-0.2119521536,2.7  
093670955\H,3.1834379306,-1.3895800175,3.087612914\O,-5.1515283277,-3.  
1706278222,-2.6814533657\O,-6.3053657611,-1.2276775705,-2.534101031\\\V  
ersion=EM64L-G09RevB.01\State=1-A\HF=-1291.1785021\RMSD=9.299e-09\RMSF  
=4.319e-06\Dipole=8.4679461,3.0653058,3.7486908\Quadrupole=-53.1709238  
,28.4214259,24.7494979,-29.7353715,-44.6697781,-16.3692525\PG=C01 [X(C  
26H34N1O3)]\\@

**18 (core)**

1\1\GINC-R2558\FOpt\UM062X\Gen\C2H7N1O4P1(2)\ROOT\12-Sep-2013\0\\#M062  
X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=5368709  
12\\hsg1\_rcore+.freq\\0,2\N,0.8032307372,0.4791694305,1.5110618537\O,-  
0.2173976289,0.6480463208,0.7605102267\c,1.7990770381,-0.4856680878,1.  
0547298779\c,1.2187050617,1.5922671438,2.3589379657\H,1.7627437996,1.2  
051023672,3.223160851\H,1.8626368001,2.2693929799,1.7846422239\H,0.313  
8006464,2.1082465741,2.6778816411\H,2.6053499715,-0.5590557075,1.78774  
96762\H,1.3175837101,-1.4599371817,0.9300515027\P,2.4602258146,0.10677  
0262,-0.5512087022\O,3.1205273814,1.4249660139,-0.4386959953\O,3.41508  
34223,-1.0798159673,-1.0637861834\H,4.3052419843,-0.7467663813,-1.2622  
212898\O,1.2118595005,-0.047170952,-1.5329559293\H,0.3898787609,0.2677  
181854,-1.0983677188\Version=EM64L-G09RevC.01\State=2-A\HF=-777.22160  
52\S2=0.755168\S2-1=0.\S2A=0.750017\RMSD=7.720e-09\RMSF=1.388e-05\Dipo  
le=0.5546122,-0.5926616,1.268929\Quadrupole=-0.3091761,-2.344038,2.653  
2142,-3.1400759,-0.3291895,1.1754558\PG=C01 [X(C2H7N1O4P1)]\\@

**18**

1\1\GINC-R319\FOpt\UM062X\Gen\C9H21N1O4P1(2)\ROOT\13-Sep-2013\0\\#M062  
X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=8053063  
68\\hsg1\_r+.freq\\0,2\N,0.8725320938,0.5254326839,1.453158451\O,-0.176  
8756379,0.610795096,0.7259958278\c,1.8318228399,-0.535617586,1.1119466  
133\c,1.1055312907,1.6496192114,2.4141578878\c,2.4124830179,1.45751297  
95,3.178072468\H,2.6437174991,-0.4793788669,1.8395641179\H,2.415403591  
3,0.5297172604,3.7617559875\H,2.5167146912,2.2879188879,3.8828134803\c  
, -0.0853425193,1.6609474395,3.3767201744\c,1.1623506353,2.9457511594,1  
.5967849601\P,2.5997455253,0.0285850947,-0.4728662515\c,1.2192834345,-  
1.9671961746,1.2045386443\H,0.00011014654,2.5162015239,4.0541588697\c,2  
.3792489839,-2.9591825046,1.3825362449\H,-0.1113408579,0.7444569657,3.  
976056779\c,0.3289753245,-2.0243793462,2.4537697933\H,-1.0223550432,1.  
7450382904,2.8207453159\c,0.3986692549,-2.371513051,-0.0267807533\H,1.  
3046333604,3.7947211087,2.2732359565\H,1.9970237384,2.9136891467,0.889  
1103328\H,0.2282018607,3.0883056335,1.047628406\H,3.2771373626,1.47750  
42723,2.5065611572\H,1.9801017537,-3.9745002215,1.4802634379\H,3.05721  
56847,-2.9441182621,0.5252555144\H,2.9543530888,-2.7378341063,2.290191  
1377\H,-0.0031741073,-3.054877586,2.6197633287\H,0.8776711124,-1.70084  
40121,3.3480647777\H,-0.5569712032,-1.3920492638,2.3431147813\H,-0.004  
5137321,-3.3782959414,0.1316083355\H,-0.4411230647,-1.6910889011,-0.18  
91431107\H,1.0130938147,-2.3960731802,-0.932441773\O,3.5093369045,1.17  
56811254,-0.2422573948\O,3.3495763121,-1.239785417,-1.1296396209\O,1.3  
742643761,0.2300024689,-1.4713676732\H,4.2887339159,-1.0341272516,-1.2  
675085802\H,0.5492462325,0.4545793246,-0.9825176236\Version=EM64L-G09  
RevC.01\State=2-A\HF=-1052.2951265\S2=0.754868\S2-1=0.\S2A=0.750017\RM  
SD=6.590e-09\RMSF=4.889e-06\Dipole=0.1396345,-0.6705614,1.3310241\Quad  
rupole=-0.3996761,1.0529072,-0.653231,-3.9419448,-0.5006011,3.6336301\  
PG=C01 [X(C9H21N1O4P1)]\\@

**18-P (core)**

1\1\GINC-V1306\FOpt\RM062X\Gen\C6H14N1O4P1\GXG501\10-Feb-2013\0\\#M062  
X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=6710886  
40\\dsg1\_core.freq\\0,1\N,0.7691077146,-0.2632278533,1.5283728726\c,0.  
1740222126,0.6664605628,0.5598629369\c,-0.0704649601,-1.4268318039,1.7  
891738639\O,1.9827592214,-0.7713545564,0.9664423074\c,3.0981105178,0.0  
529595316,1.321422663\H,2.8137199985,1.101300824,1.155210692\c,4.20993  
66076,-0.3177148484,0.3476136077\c,3.5248668727,-0.1401205137,2.752421  
8584\H,3.9057882066,-0.0780054132,-0.6746816045\H,4.435129372,-1.38542  
30345,0.4390610797\H,5.1183778457,0.2426033608,0.5879352027\H,4.181769  
0086,0.6374352762,3.1422189295\c,3.2052248025,-1.18355953,3.5126240657  
\H,2.5605019088,-1.9738894833,3.1399174852\H,3.5789742983,-1.279890831  
,4.5269689177\P,0.6486462246,0.3404406485,-1.1809018281\O,1.8845324079  
,1.0218058644,-1.629347355\O,-0.6797424152,0.7788547992,-1.980762994\H  
, -0.4556318381,1.1819735355,-2.8354093994\O,0.6127977469,-1.2581522345  
, -1.3676473632\H,1.3650120391,-1.6475520851,-0.8825241057\H,0.49845099  
95,1.690427487,0.776239956\H,-0.9152797891,0.6354404212,0.6535989202\H  
, -0.3072300481,-2.0020604959,0.8831445504\H,-0.9976175005,-1.070101775

3,2.2438190488\H,0.4436365454,-2.0674908528,2.506678692\\Version=EM64L  
-G09RevB.01\State=1-A\HF=-933.7821214\RMSD=7.184e-09\RMSF=3.654e-06\Di  
pole=-0.4121201,-0.0818757,0.6488951\Quadrupole=0.7255617,0.1276903,-0  
.8532519,-1.5933242,1.9375275\PG=C01 [X(C6H14N1O4P1)]\\@

**18-P**

1\1\GINC-R90\FOpt\RM062X\Gen\C25H38N1O4P1\ROOT\16-Sep-2013\0\\#M062X/g  
en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280  
\dhsg1.freq\0,1\N,-1.4486582637,0.6115762853,-0.7989918238\O,-0.6379  
218333,0.9048761077,0.3435062146\C,0.7486085437,0.5039724102,0.2491913  
554\C,-2.5224136896,-0.3259842485,-0.3822216484\C,-1.905680809,1.91302  
11978,-1.3961563193\C,-2.7114022609,1.6200188529,-2.6674757267\H,-3.48  
23323592,0.067828489,-0.7398190385\H,-2.1189616435,1.0522091767,-3.388  
9232556\H,-2.9813601789,2.5756753327,-3.1269707974\C,-0.6587658867,2.6  
942696767,-1.8157854088\C,-2.7475958773,2.7770853153,-0.4496291302\P,-  
2.7829027517,-0.4164743538,1.4561102316\C,-2.3620717262,-1.747978781,-  
1.0187880539\C,1.0355881809,-0.3544107038,1.484065517\C,2.498360196,-0  
.8037190808,1.6215006316\C,2.6754372252,-1.6113069727,2.913788984\C,1.  
6441655792,1.7234159529,0.19990775\C,2.5901450183,1.8745774062,-0.8133  
587342\C,3.4239998421,2.9929227529,-0.844997558\C,3.3129165165,3.97434  
72177,0.1377235153\C,2.3686112603,3.8300899961,1.1557014674\C,1.544979  
4279,2.7081666563,1.187925015\C,2.9713168235,-1.5942132817,0.415378920  
4\C,4.0800036379,-1.1754593421,-0.3255097025\C,4.5202255701,-1.8999119  
885,-1.433718196\C,3.8529832877,-3.0607984883,-1.8186248504\C,2.749891  
3469,-3.4946579681,-1.0827523471\C,2.3178737466,-2.7693442529,0.024954  
343\H,-0.9560795716,3.542814379,-2.4406430485\C,-3.5283718696,-2.65207  
26529,-0.5883665275\H,0.017831031,2.0570661429,-2.3958670518\C,-2.3976  
759371,-1.6211307614,-2.5465035815\H,-0.1158756922,3.0855591772,-0.953  
9414793\C,-1.0391518217,-2.4124468269,-0.6305559899\H,-3.0530320725,3.  
6874242638,-0.9766739916\H,-3.6527496072,2.2660537715,-0.1064100977\H,  
-2.171697631,3.0830336237,0.427896665\H,0.3635502063,-1.2186067947,1.4  
767832316\H,0.7618346166,0.228173761,2.3755183161\H,0.8663710763,-0.07  
37281775,-0.672867319\H,2.6706331704,1.1123286368,-1.5857401132\H,4.15  
43499435,3.1000506396,-1.6420829737\H,3.9569955133,4.8484090303,0.1118  
09959\H,2.275934239,4.5921748152,1.9241696703\H,0.8074449142,2.6029029  
944,1.9812852253\H,3.1273318502,0.0936856035,1.6927587155\H,4.59988490  
62,-0.2655612108,-0.0319239228\H,5.3847084446,-1.5562246816,-1.9951320  
081\H,4.1909218494,-3.6261191749,-2.6822594931\H,2.2244772915,-4.40102  
88334,-1.3713014488\H,1.4575374313,-3.1209830828,0.5907717332\H,2.3873  
131737,-1.0133491203,3.7849112055\H,3.7165080532,-1.9256007066,3.03623  
49791\H,2.0485053274,-2.5095826673,2.9019457127\H,-3.6433856091,1.0811  
489047,-2.4769117383\H,-3.4942035179,-3.5809216587,-1.1683305843\H,-3.  
463366261,-2.9237246036,0.4696759919\H,-4.498683342,-2.1747292517,-0.7  
682774194\H,-2.2933688989,-2.6160224627,-2.9936224684\H,-3.3433485332,  
-1.193991045,-2.8996121238\H,-1.5721396558,-1.0011155802,-2.9064398692  
\H,-0.9581600498,-3.3829551034,-1.1356808758\H,-0.1876676751,-1.807088  
2368,-0.9545932254\H,-0.9784772571,-2.5782902162,0.4477549907\O,-2.042  
7269583,-1.4741147486,2.1863169573\O,-2.6476648675,1.0722457491,2.0382  
350985\O,-4.3888926136,-0.594294754,1.5411285149\H,-1.7564338229,1.408  
9537444,1.8236961006\H,-4.6195246959,-1.2458942493,2.2226319292\\Version=EM64L-G09Rev  
C.01\State=2-A\HF=-776.7000179\S2=0.755558\S2-1=0.\S2A=0.750021\RMSD=6  
.366e-09\RMSF=9.314e-06\Di pole=-1.510205,0.1945202,2.0615651\Quadrupole  
=-7.869087,2.5226914,5.3463957,0.7728629,5.7490459,-1.7516524\PG=C01  
[X(C2H6N1O4P1)]\\@

**18- (core)**

1\1\GINC-R1683\FOpt\UM062X\Gen\C2H6N1O4P1(1-,2)\ROOT\12-Sep-2013\0\\#M  
062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=5368  
70912\hsg1c\_rcore+.freq\0,-1,2\N,0.7739522518,0.5243926726,1.554184418  
4\O,-0.24870784,0.5443398798,0.7820633434\C,1.900146275,-0.3235178267,  
1.1848798162\C,1.0393998728,1.7292969853,2.3304949087\H,1.625104376,1.  
4647910137,3.216320697\H,1.6113679548,2.4305392669,1.7105019982\H,0.07  
44405939,2.1470046916,2.6227188244\H,2.5825522898,-0.3908685986,2.0377  
414907\H,1.5108681212,-1.3154793882,0.9409029027\P,2.8331869277,0.3660  
404313,-0.2910262758\O,1.688311285,0.1004919564,-1.4552027351\H,0.8738  
591944,0.5671345128,-1.1986757214\O,2.9601265862,1.8455418431,-0.03506  
20945\O,3.9890031115,-0.5442934399,-0.5641165731\\Version=EM64L-G09Rev  
C.01\State=2-A\HF=-776.7000179\S2=0.755558\S2-1=0.\S2A=0.750021\RMSD=6  
.366e-09\RMSF=9.314e-06\Di pole=-1.510205,0.1945202,2.0615651\Quadrupole  
=-7.869087,2.5226914,5.3463957,0.7728629,5.7490459,-1.7516524\PG=C01  
[X(C2H6N1O4P1)]\\@

**18-**

```
1\1\GINC-R423\FOpt\UM062X\Gen\C9H20N1O4P1(1-,2)\ROOT\13-Sep-2013\0\\#M
062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=8053
06368\hsglc_r+.freq\~-1,2\N,0.811531798,0.6001601457,1.4749643744\O,-
0.2232577096,0.5878900861,0.7182721335\c,1.8762526904,-0.3742936461,1.
2053801088\c,0.9222299389,1.7781321997,2.3832714361\c,2.2348682684,1.7
675536177,3.1633016797\h,2.5901301216,-0.2854827345,2.028126123\h,2.31
59501248,0.8871772,3.8120745697\h,2.2553667928,2.6557126779,3.80543482
89\c,-0.2713207048,1.7061374464,3.3436316127\c,0.8495541826,3.04767248
86,1.5249877447\P,2.8579526769,0.2206421322,-0.2996271311\c,1.36128831
99,-1.8412132433,1.2212378733\h,-0.2789831849,2.5879515722,3.994908418
4\c,2.5770907632,-2.7450762134,1.4803352706\h,-0.2096964965,0.80891566
4,3.9708807314\c,0.3598843653,-2.0179044265,2.3718529334\h,-1.20614917
76,1.672684076,2.777070819\c,0.7070359995,-2.2747323835,-0.0973138749\
h,0.8978228561,3.9302436783,2.1746079948\h,1.6923859917,3.0561238639,0
.8261649721\h,-0.0916914206,3.0700645656,0.9685078582\h,3.0855350579,1
.8082925466,2.4752609748\h,2.2655157649,-3.798032604,1.4704106063\h,3.
3390954178,-2.585021199,0.7113251261\h,3.0197741686,-2.5338274517,2.46
35799786\h,0.0950086445,-3.0781310272,2.4778683638\h,0.7939583368,-1.6
81849173,3.3242663275\h,-0.5570326187,-1.4471997746,2.1914624404\h,0.3
590274658,-3.3130115424,-0.0014207854\h,-0.1460235343,-1.6362542246,-0
.340393727\h,1.4262040999,-2.2178476165,-0.9195474769\o,3.3151380892,1
.5996801685,0.1039250866\o,3.7973207152,-0.8619582858,-0.737669291\o,1
.6619417184,0.3274363102,-1.4303119119\h,0.8799914778,0.7651131065,-1.
0486961885\Version=EM64L-G09RevC.01\State=2-A\HF=-1051.7737034\S2=0.7
55137\S2-1=0.\S2A=0.750019\RMSD=9.703e-09\RMSF=8.867e-06\Dipole=-2.095
8946,-0.0167498,2.8856689\Quadrupole=-5.105336,4.2255246,0.8798114,-0.
7179173,9.9685057,-0.4655905\PG=C01 [X(C9H20N1O4P1)]\@
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**18<sup>-</sup>P (core)**

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1\1\GINC-R96\FOpt\RM062X\Gen\C6H13N1O4P1(1-)\ROOT\15-Sep-2013\0\\#M062
X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=8053063
68\dhsglc_core.freq\~-1,1\N,-1.8992133712,0.9934956237,0.0698747282\c
,-0.7370328057,1.3533770302,0.8713314546\c,-1.5131952353,0.5003463749,
-1.2726104059\o,-2.6271485969,2.2292987779,-0.0484655742\c,-3.98470419
4,1.988469356,-0.3781502193\h,-4.0241008609,1.2723016943,-1.2101775138
\c,-4.5278820052,3.3182545488,-0.8909027647\c,-4.7911958907,1.47947506
8,0.7884216946\h,-4.3935793237,4.0922330757,-0.1262949244\h,-3.9904913
48,3.5734110239,-1.8082880834\h,-5.5974950383,3.2310677972,-1.11245666
07\c,-4.3565683008,1.3578413261,2.0407848093\h,-5.8245850097,1.2219164
753,0.5471956227\h,-3.3272126588,1.5924530759,2.294255091\h,-5.0078343
076,1.0057411662,2.8364583212\h,-0.0918923584,2.0905915621,0.373215634
9\h,-0.1671415249,0.4389452703,1.0586660674\h,-1.0833907804,1.75396779
73,1.8289165126\h,-0.5842529212,-0.0645588182,-1.1482798766\h,-2.27633
62757,-0.2093498192,-1.6154889045\P,-1.2661206853,1.7312204054,-2.6607
230685\o,-0.2447645973,1.1454914134,-3.5865978278\o,-2.6383224009,2.17
73600323,-3.103312806\o,-0.5553416945,2.9922097742,-1.841855688\h,-1.2
686628146,3.4165949683,-1.335476619\Version=EM64L-G09RevC.01\State=1-
A\HF=-933.2531187\RMSD=4.765e-09\RMSF=7.016e-06\Dipole=-1.7348696,-0.1
054333,3.4918154\Quadrupole=1.5913005,9.8729581,-11.4642586,0.9413959,
12.6312037,-0.410464\PG=C01 [X(C6H13N1O4P1)]\@
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**18<sup>-</sup>P**

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1\1\GINC-R93\FOpt\RM062X\Gen\C25H37N1O4P1(1-)\ROOT\16-Sep-2013\0\\#M06
2X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=134217
7280\dhsglc.freq\~-1,1\N,1.7264795019,0.7526527725,0.1761343557\o,0.8
12782735,0.7961795893,-0.9387298649\c,-0.538620517,0.5370878028,-0.560
1617682\c,2.3595968696,-0.6029856423,0.2980755971\c,2.6702915049,1.888
429757,-0.0833511876\c,3.6857054496,2.0110468564,1.058744442\h,3.4471
352117,-0.4628893168,0.2541219938\h,3.1884255972,2.1862611175,2.016007
5913\h,4.3303833815,2.8712220523,0.8468618602\c,1.8557119655,3.1865263
137,-0.094486701\c,3.4345290185,1.7615717368,-1.4103454915\P,2.0881448
219,-1.8193664285,-1.1399509514\c,2.0755424746,-1.2625026312,1.6969326
592\c,-1.2358674058,0.0920834054,-1.8468065383\c,-2.7505260186,-0.1170
953691,-1.703506233\c,-3.3085048553,-0.736816265,-2.992805443\c,-1.204
3419154,1.7410522957,0.0795089112\c,-1.685700616,1.6781539211,1.387201
0358\c,-2.318064297,2.7773560719,1.9715371193\c,-2.4805956553,3.955653
042,1.2472804546\c,-2.0168807442,4.0249304541,-0.0687276306\c,-1.39054
37993,2.9239491438,-0.6444885214\c,-3.1357318842,-0.9714317053,-0.5087
019361\c,-4.2681932234,-0.642768253,0.2434802063\c,-4.663729955,-1.423
9055312,1.3281620306\c,-3.9206478096,-2.5505768536,1.6789653093\c,-2.7
860744773,-2.8825590428,0.9385585078\c,-2.3934543833,-2.1041810483,-0.
1505542457\h,2.5365078872,4.0462778781,-0.0966800647\c,2.9179017726,-2
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.542155141,1.8384956311\H,1.2139933143,3.24486888,0.7919601632\C,2.470
7503192,-0.3219493133,2.8440481008\H,1.2230602148,3.2494700591,-0.9809
807835\C,0.6025952444,-1.6325064083,1.9166181828\H,4.1130684566,2.6173
526476,-1.5165363928\H,4.0200444751,0.8395477898,-1.4634480179\H,2.747
5033464,1.7640631456,-2.260001253\H,-0.7450631879,-0.8383353123,-2.156
8279011\H,-1.0621425073,0.8432391067,-2.6311862832\H,-0.5427600318,-0.
3000369824,0.1380366745\H,-1.5747332393,0.7536932246,1.9485891045\H,-2
.6837179716,2.7093020243,2.992793646\H,-2.9694059492,4.8143087823,1.70
03323023\H,-2.1452459376,4.9385678586,-0.6437250602\H,-1.0277962418,2.
981335815,-1.6687813268\H,-3.2254795492,0.8645972031,-1.564308488\H,-4
.8341848308,0.2511760559,-0.0148304055\H,-5.542230963,-1.1455879194,1.
9053236319\H,-4.2158296514,-3.1576509018,2.5310457912\H,-2.184379796,-
3.7441155204,1.2162686852\H,-1.4755697946,-2.3545790146,-0.6860436009\
H,-3.0631561052,-0.1132788018,-3.8609266119\H,-4.3973593671,-0.8452797
305,-2.9379171\H,-2.8732240616,-1.7295747924,-3.1519505822\H,4.3300302
355,1.133949848,1.1525326539\H,2.8522601052,-2.8993705067,2.8753448905
\H,2.5806925142,-3.3332661554,1.165638761\H,3.9709932989,-2.3540513709
,1.5989330155\H,2.2261875836,-0.7995149791,3.8020839308\H,3.5457365716
,-0.1072508691,2.846494653\H,1.9180355254,0.6210853462,2.7842001502\H,
0.5103827649,-2.2134105217,2.8445417784\H,-0.0105004968,-0.733244222,2
.0381249173\H,0.2134917469,-2.2241995056,1.084563978\O,3.2307750697,-2
.785965272,-1.1012840375\O,0.6423522264,-2.2660871203,-1.1196708532\O,
2.3296794148,-0.8570509328,-2.4561371795\H,1.6099796194,-0.2039216163,
-2.4669422616\"Version=EM64L-G09RevC.01\State=1-A\HF=-1671.4794213\RMS
D=6.909e-09\RMSF=2.951e-06\Di pole=-2.8977064,3.6232595,1.6212822\Quadr
upole=-9.0982254,-2.7921518,11.8903772,13.8756938,7.8844847,-12.062607
2\PG=C01 [X(C25H37N1O4P1)]\\@
```

**18<sup>2-</sup>** (core)

```

1\1\GINC-V1356\FOpt\UM062X\Gen\C2H5N1O4P1(2-,2)\GXG501\09-Mar-2013\0\\
#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm max
disk=671088640\\sgla_rcore+.freq\\-2,2\N,-1.4366924267,0.5545218877,-0
.7059960859\C,-0.7973251501,0.275595495,-1.9815478071\C,-2.5636384651,
-0.2521520117,-0.2245560067\H,-0.7778457665,-0.8095143852,-2.128255756
8\H,-1.3812066601,0.7224885872,-2.7968770296\H,0.2064177381,0.71371726
39,-1.9400519188\H,-2.2975114449,-0.6148049716,0.7782732777\H,-3.42152
66732,0.4272335454,-0.1268567056\P,-3.0858619541,-1.7436459197,-1.3074
142399\O,-1.802594065,-2.6002529639,-1.3697048471\O,-4.2374012008,-2.3
16485053,-0.4693699524\O,-3.4726021777,-1.079358921,-2.6418966794\O,-1
.1348447539,1.6589144469,-0.1187892483\"Version=EM64L-G09RevB.01\HF=-7
75.98936\S2=0.755616\S2-1=0.\S2A=0.750022\RMSD=8.344e-09\RMSF=2.829e-0
5\Di pole=1.7399616,1.998878,0.1865003\Quadrupole=-29.4643814,6.755319,
22.7090624,-35.239926,-26.9832401,-14.9333575\PG=C01
[X(C2H5N1O4P1)]\\@
```

**18<sup>2-</sup>**

```

1\1\GINC-V1257\FOpt\UM062X\Gen\C9H19N1O4P1(2-,2)\GXG501\10-Mar-2013\0\
#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm ma
xdisk=671088640\\sgla_r+.freq\\-2,2\N,-1.7299973673,0.5625662207,-1.25
31366792\O,-0.5830676844,0.2488721691,-1.7410337879\C,-2.496254544,-0.
3684797003,-0.4254202395\C,-2.1273855541,1.9783052668,-1.4738040199\C,
-2.196557068,2.1856901893,-2.9958026983\H,-3.5463105167,-0.0993814727,
-0.5824911192\H,-1.232277471,1.9373985214,-3.4498322552\H,-2.447797659
7,3.2310943579,-3.2223761095\C,-1.0479405908,2.8791783109,-0.858446871
4\C,-3.4820043894,2.3084667304,-0.8442760973\P,-2.3726309624,-0.080951
4857,1.5481386498\C,-2.3636202578,-1.8337166825,-0.9162578483\H,-1.298
0008232,3.9347192285,-1.0432481648\C,-3.4048574153,-2.6624585857,-0.14
60597797\H,-0.0778307947,2.6533632789,-1.3130814132\C,-2.6891650166,-1
.9096001575,-2.419132527\H,-1.0143587855,2.6684586808,0.2175975407\C,
-0.9837894597,-2.4653861587,-0.6646029309\H,-3.6742515927,3.3795811797,
-1.0005169193\H,-4.297694733,1.7483947255,-1.3177838954\H,-3.460794595
2,2.0971806624,0.2308493667\H,-2.966745446,1.5371815729,-3.4342993653\
H,-3.4024544941,-3.6969182645,-0.5271304287\H,-3.1714772495,-2.6589755
65,0.9229035987\H,-4.4123122987,-2.2425340439,-0.2613134558\H,-2.66106
00796,-2.9553063573,-2.7659932299\H,-3.6959840992,-1.5127851842,-2.619
0494663\H,-1.9627621207,-1.3304620772,-3.0005864607\H,-1.0356713811,-3
.5439999179,-0.8931904309\H,-0.221162403,-2.0024148414,-1.2953098178\H
,-0.7212676194,-2.3209117889,0.3894544945\O,-1.4330408751,-1.175482639
,2.0635495819\O,-1.8541529628,1.3615013183,1.6480583804\O,-3.858371689
8,-0.2622074911,1.8956343989\"Version=EM64L-G09RevB.01\HF=-1051.067022
1\S2=0.755847\S2-1=0.\S2A=0.750026\RMSD=9.339e-09\RMSF=5.065e-06\Di pol
e=-0.4673985,0.6716877,-4.6387813\Quadrupole=-13.5944739,13.8241179,-0
```

.229644,-3.1855618,19.9014846,1.4673597\PG=C01 [X(C9H19N1O4P1)]\\@

**18<sup>2-</sup>-P** (core)

```
1\1\GINC-X147\FOpt\RM062X\Gen\C6H12N1O4P1(2-)\GXG501\27-Feb-2013\0\\#M
062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdi
sk=536870912\dsbla_core.freq\-\2,1\N,-0.6025316091,0.5205961649,-0.74
34284363\O,-0.0266111307,1.1929104095,0.411179131\C,0.3929954025,0.837
5008166,-1.7678506299\C,-1.9128481328,1.1296966449,-1.1047619302\C,-0.
8214326328,1.0779266385,1.5632148186\H,-1.8657770522,1.3157969442,1.31
72845636\C,-0.3587096583,2.2014267378,2.4875861341\C,-0.7177436351,-0.
2754107654,2.2209157264\H,0.7192233709,2.1149037504,2.6799531376\H,-0.
6076131192,3.132159706,1.9656218458\H,-0.896233739,2.1590551957,3.4447
828317\C,0.0215786908,-1.2948990557,1.779813807\H,-1.3081268293,-0.390
9595087,3.1352781041\H,0.0563233503,-2.2474809911,2.3073170384\H,0.574
2523913,-1.1938604696,0.849665961\H,0.0932067433,0.3211217352,-2.68737
15619\H,0.4366425403,1.9222520764,-1.9476364325\H,1.3638176893,0.44177
45921,-1.4391170993\H,-2.0868903831,0.8134106358,-2.1414316993\P,-2.20
93466715,3.0253135106,-1.0693175267\H,-2.6913169538,0.6361341087,-0.50
37512446\O,-1.0033776963,3.6045243561,-1.8338642188\O,-3.5620042198,3.
0909664475,-1.8004043293\O,-2.2672257156,3.3772413197,0.4347170093\V
ersion=EM64L-G09RevB.01\HF=-932.5354872\RMSD=4.125e-09\RMSF=1.151e-05\Di
pole=2.6074781,-4.0849805,2.6729747\Quadrupole=2.1949692,-27.3939935,
25.1990244,44.3231771,-17.7120845,22.7631176\PG=C01 [X(C6H12N1O4P1)]\\
```

**18<sup>2-</sup>-P**

```
1\1\GINC-V1476\Freq\RM062X\Gen\C25H36N1O4P1(2-)\GXG501\18-Mar-2013\0\\
#M062X/gen 6D SCF=Tight INT(grid=ultrafine) Freq=Noramian IOP(2/17=4) m
axdisk=2013265920\dsbla.freq\-\2,1\N,0.7883677204,0.7612235782,1.4377
771786\O,0.1251589004,1.0790351915,0.1879027625\C,-1.0237692383,0.3201
77325,-0.0978181028\C,1.4612823374,-0.5844524675,1.4051448708\C,1.7506
953814,1.9036783019,1.5275248853\C,2.4413555534,1.9045535824,2.8959665
192\H,2.5058303179,-0.4141373493,1.688775482\H,1.7120466053,2.00014732
6,3.7085086553\H,3.1243737921,2.763309313,2.9365099939\C,0.951429062,3
.2143700459,1.4402419172\C,2.8084241092,1.8752694577,0.4106195505\P,1.
7980955283,-1.5288217771,-0.3044491235\C,0.8875457019,-1.5044956856,2.
5406124238\C,-1.1223397361,0.4163812552,-1.6319637653\C,-2.4537196681,
0.0193167729,-2.2819370857\C,-2.3136413382,0.1268150863,-3.8097102548\
C,-2.2669024073,0.868526461,0.586549707\C,-3.299275507,0.019986646,1.0
007625996\C,-4.4784019834,0.5361927346,1.538297147\C,-4.6423641294,1.9
143790646,1.6805758227\C,-3.6147137107,2.7696555642,1.2782442133\C,-2.
4418371281,2.2482352452,0.7342606345\C,-2.9703956862,-1.3630560321,-1.
9235068751\C,-4.3497817266,-1.6100466966,-1.9635248264\C,-4.8687568333
,-2.8637106503,-1.6463420304\C,-4.0038475724,-3.8968521107,-1.27543135
18\C,-2.630926297,-3.6569309546,-1.2332588412\C,-2.1072081944,-2.40353
088,-1.5636499264\H,1.5865519891,4.0549482199,1.7518698143\C,1.6710380
805,-2.8254566103,2.5872699852\H,0.0794170962,3.1633749442,2.103977499
6\C,1.0289230734,-0.8328048764,3.9183188595\H,0.6079019222,3.398993615
7,0.4196897543\C,-0.5986424612,-1.8371570903,2.3610037764\H,3.33724470
78,2.840345884,0.3798932394\H,3.5439474586,1.0798188566,0.5730235672\H
,2.3374480724,1.6528974675,-0.5517757798\H,-0.2628460692,-0.1570834276
,-2.0101130019\H,-0.9304021667,1.4685134,-1.8931964149\H,-0.8640018999
,-0.7282955881,0.1694958383\H,-3.1729986482,-1.055995101,0.8958353471\
H,-5.2690571141,-0.1432245379,1.8496779036\H,-5.5593494805,2.318144550
6,2.1052808855\H,-3.728222841,3.8464689447,1.3900281761\H,-1.634555842
5,2.904417015,0.4212386947\H,-3.2257695152,0.7390117113,-1.9650224529\
H,-5.0262638588,-0.7935487842,-2.2185682758\H,-5.9446682234,-3.0290866
143,-1.669705634\H,-4.4027863748,-4.8731998193,-1.0061404672\H,-1.9360
597339,-4.4318260991,-0.9184604254\H,-1.0220028751,-2.2608154749,-1.44
93583718\H,-1.9869832682,1.1337504016,-4.0979815487\H,-3.2635185711,-0
.0925497514,-4.3136189621\H,-1.5620326605,-0.5877645503,-4.1633002185\
H,3.0318639777,1.001323265,3.0622814985\H,1.3434975195,-3.406389367,3.
4659346304\H,1.506370933,-3.4045670927,1.6754614804\H,2.7495989987,-2.
6432327625,2.655329186\H,0.5958765269,-1.4795665389,4.6971979467\H,2.0
831767904,-0.6645715757,4.1758016816\H,0.5032326779,0.1281856726,3.938
1302403\H,-0.927985618,-2.5013493078,3.1757653359\H,-1.2060912701,-0.9
255920421,2.4116137669\H,-0.7509114359,-2.3453006845,1.4024381559\O,0.
5730394151,-2.4684241657,-0.4396985159\O,1.8763753564,-0.4613658758,-1
.3967933364\O,3.1111834796,-2.2251375587,0.057060962\Version=EM64L-G0
9RevB.01\State=1-A\HF=-1670.7859416\RMSD=8.597e-09\RMSF=2.123e-05\Zero
Point=0.5752289\Thermal=0.6064574\Di pole=-5.6291878,3.018426,1.2791508
\PG=C01 [X(C25H36N1O4P1)]\\@
```

7 (core)

```
1\1\GINC-D20\FOpt\UM062X\Gen\C9H10N1O3(2)\ETS502\01-Sep-2013\0\#M062X
/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdisk=1
610612736\tncl_r+core.freq\0,C,2.6103283958,-0.9316864097,0.283335
8567\N,1.511240186,-0.9565490658,-0.6726821326\O,1.0130023476,0.160183
7466,-1.0330339361\C,0.640727685,-2.132046491,-0.7068723755\H,3.288589
5306,-0.1312334295,-0.0125151811\H,-0.0240612487,-1.9818093306,-1.5611
293815\C,-0.1436198165,-2.2898012042,0.5796708784\C,-0.9545098086,-1.2
416173485,1.0302130092\C,-1.6653825647,-1.3663494484,2.218083082\C,-1.
5709141546,-2.5456332576,2.964707006\C,-0.7623009804,-3.5929586476,2.5
229468453\C,-0.0489398392,-3.4601250321,1.3354555101\C,-2.3138212994,-
2.7292374163,4.2405282621\O,-2.2674708009,-3.7221811311,4.928419916\O,
-3.0650357911,-1.6591960485,4.5715983403\H,2.2320005432,-0.7381756054,
1.2950912176\H,3.1284569408,-1.8938651519,0.2679095121\H,1.2585266558,
-3.0180433808,-0.8875170128\H,-1.0149072077,-0.3267641454,0.4457136547
\H,-2.2952078101,-0.5562041289,2.5700809087\H,-0.700885146,-4.4977862
692,3.1197553867\H,0.585179798,-4.2741604379,0.9920626159\H,-3.5085922
465,-1.872396366,5.4106160179\Version=EM64L-G09RevC.01\HF=-629.10378\S2=0.755136\S2-1=0.\S2A=0.750015\RMSD=5.646e-09\RMSF=5.316e-06\Dipole=0.4301414,-0.4656303,0.0742738\Quadrupole=5.9390421,-2.3069045,-3.6321
377,-6.8233593,-0.824039,9.1882141\PG=C01 [X(C9H10N1O3)]\\@
```

7

```
1\1\GINC-R2131\FOpt\UM062X\Gen\C15H22N1O3(2)\ROOT\29-Aug-2013\0\#M062
X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdisk=
2147483648\tncl_r+.freq\0,N,1.4890990187,-0.9328088463,-0.61248645
83\O,0.9327594833,0.1816368359,-0.882285473\C,3.6881500478,0.086965641
1,-0.5644844391\C,-0.2505744294,-2.0910720597,-1.932065154\C,2.7524888
114,-0.8689429664,0.1798429641\C,0.6352628698,-2.1365789956,-0.6733851
705\C,2.4347725291,-0.323234708,1.5782930711\C,-0.160815536,-2.2864014
715,0.6112448278\C,3.3962137168,-2.2508204648,0.2786658033\H,2.7920297
252,-2.9468563672,0.8696151397\H,4.3631346551,-2.1485667921,0.78073298
76\H,3.3659000114,-0.1619092884,2.1320947532\H,1.81176183,-1.021661785
7,2.1464071501\H,1.9060140499,0.6306830858,1.4935978831\H,3.9000360156
,-0.2909372858,-1.5706178759\C,-1.1094483379,-3.3545715153,-2.01121769
43\H,3.2336627479,1.0755947157,-0.6537622838\C,0.6130766943,-1.9419380
52,-3.1851121773\H,4.6322331694,0.1761395113,-0.0178928752\H,-0.904193
6845,-1.2153955202,-1.8461413505\H,3.5757317431,-2.6811206247,-0.71311
89896\H,1.3012686663,-3.0000581149,-0.7735399214\H,-0.4798573515,-4.25
35618854,-2.0477153422\H,-1.717946412,-3.3396930787,-2.9208578453\H,-1
.7840605413,-3.4490014061,-1.1549838434\H,1.3196316256,-2.7788784556,-
3.2670911726\H,1.1803208113,-1.0080135488,-3.1707805912\H,-0.014087797
3,-1.9483434767,-4.0824806838\C,-0.9710759238,-1.2401932073,1.06796662
36\C,-1.6964170348,-1.3767619981,2.245954555\C,-1.6205794641,-2.566303
3376,2.978237008\C,-0.8194831121,-3.6159286489,2.5267118401\C,-0.09393
7283,-3.4715085396,1.3485884226\H,-1.0102408635,-0.3121513214,0.503448
8506\H,-2.3204172967,-0.5646745326,2.6041428958\C,-2.3752394793,-2.759
8148533,4.2445800344\H,-0.7751148938,-4.5317371984,3.1082202752\H,0.53
03004371,-4.2897483381,0.9950014561\O,-3.1183342814,-1.6866502149,4.58
60359308\O,-2.3454808141,-3.762381067,4.919900841\H,-3.5696701229,-1.9
088228227,5.4184510284\Version=ES64L-G09RevD.01\HF=-864.8828285\S2=0.
754738\S2-1=0.\S2A=0.750014\RMSD=6.528e-09\RMSF=1.376e-05\Dipole=0.538
1834,-0.2505118,-0.1922293\Quadrupole=6.6955381,-3.6410572,-3.0544809,
-6.4787501,-0.2940772,9.3886928\PG=C01 [X(C15H22N1O3)]\\@
```

7-P (core)

```
1\1\GINC-R344\FOpt\RM062X\Gen\C13H17N1O3\ROOT\02-Oct-2013\0\#M062X\ge
n 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdisk=2147
483648\pstnclcore.freq\0,1\N,0.5519721598,0.23713085,-0.1912941977\C
,1.8111774461,0.0871711698,-0.9073489624\C,0.4114955892,1.5675366465,0
.3985316624\O,0.5960006945,-0.66849617,0.9033372708\C,-0.504089808,-1.
5791546125,0.8250996601\C,-0.3303031059,-2.5323458595,-0.3250826\C,-1.
1629900631,-2.6100047946,-1.3603509083\C,-0.5309796775,-2.3019562919,2
.163311527\C,0.1756463482,2.6113301986,-0.6677131653\C,-0.7727301052,2
.3865414932,-1.6738176644\C,-1.0120946074,3.3517898182,-2.6422258923\C
,-0.3044268347,4.55795001,-2.616590821\C,0.6452714302,4.7901811214,-1.
6208192827\C,0.8830578193,3.8145992965,-0.6554628705\C,-0.5950053916,5
.5617147545,-3.6734399173\O,-1.4031949805,5.4171109435,-4.561047776\O,
0.1441398383,6.6851069547,-3.5536648476\H,2.6763026469,0.2684028838,-0
.2506101194\H,-0.4534969968,1.5225988344,1.069961017\H,1.865483304,-0.
9262106675,-1.3096103187\H,1.8254316268,0.8005046538,-1.7358761644\H,-
0.6401808484,-1.5840952776,2.9809653069\H,-1.3652943292,-3.0082951004,
2.192182114\H,0.4010992455,-2.8568069181,2.3115608441\H,-1.4268587937,
```

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-0.9984198725,0.6812163807\H,-1.0123911107,-3.3214731813,-2.1669095867
\H,0.5434518815,-3.1838221343,-0.2647882452\H,-2.0285258146,-1.9547971
405,-1.4339470313\H,1.2923692161,1.8298775138,1.0084372995\H,-1.306934
9176,1.440490748,-1.6921960554\H,-1.7437065605,3.191203436,-3.42825966
84\H,1.1959677416,5.7248110565,-1.607819071\H,1.6287254386,3.990165354
2,0.1159626557\H,-0.1172104812,7.2732712831,-4.2828445725\\Version=ES6
4L-G09Revd.01\HF=-785.6671181\RMSD=4.601e-09\RMSF=6.492e-06\Di pole=0.3
872159,-0.1559928,0.5026858\Quadrupole=-0.5179912,6.2651288,-5.7471376
,6.1161886,-4.6558611,3.2983547\PG=C01 [X(C13H17N1O3)]\\@
```

7-P

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1\1\GINC-R96\FOpt\RM062X\Gen\C31H39N1O3\ROOT\24-Sep-2013\0\\#M062X/gen
6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdisk=34896
60928\pstnc1.freq\0,1\N,1.2285727793,0.1648713388,-0.0067358038\0,0.
7320147446,-0.8275304035,0.8854061885\c,-0.5698946096,-1.251382503,0.4
669318801\c,-1.3159184656,-1.7335675149,1.7077050932\c,-0.5210599516,-
2.2662461051,-0.6556254564\c,3.5330366151,-0.2458626425,0.9175205975\c
,0.1964216848,1.6189477752,1.8420413034\c,2.6389687077,-0.1872325087,-
0.3299664452\c,1.0488443265,1.544275019,0.5499501519\c,2.6507956822,-1
.5547038865,-1.0170825779\c,0.4759664896,2.4393262222,-0.540353322\c,3
.1663049635,0.8513773273,-1.3263013067\H,2.4738754212,0.962398921,-2.1
673759908\H,4.1339213905,0.5149315075,-1.7121189169\H,3.6678510005,-1.
7817678651,-1.3544484186\H,1.9829656658,-1.5586928773,-1.8846969679\H,
2.3319414037,-2.343721104,-0.3332651708\H,4.5528343456,-0.52466358,0.6
303674881\c,-0.2562304973,3.0552192378,2.1303512029\H,3.5872786437,0.7
17158354,1.4366838302\c,0.9756005446,1.0926219012,3.0508528302\H,3.156
9615754,-0.996201581,1.6194353858\H,-0.7062629462,1.0155899589,1.69463
43891\H,-1.1522875035,-1.0012675936,2.5097702737\c,-2.827803364,-1.881
6883074,1.4472835288\H,-0.9080044763,-2.687079298,2.0643580162\H,-1.08
97058961,-0.3695301574,0.08922704\c,-0.8842054647,-1.8870966595,-1.94
91529632\c,-0.8084982254,-2.7940321024,-3.0067001638\c,-0.3640865507,-
4.0941393129,-2.7768160776\c,-0.0000258383,-4.4833164171,-1.486470222\
c,-0.0823456628,-3.57519953,-0.4344308921\H,-1.21349888,-0.8660694609,
-2.1306007056\H,-1.0894931292,-2.4823338581,-4.008669927\H,-0.29990380
48,-4.8024863118,-3.5977619715\H,0.3508221046,-5.4948752835,-1.3025522
21\H,0.2223212381,-3.8811065976,0.5640512397\H,-2.9629916069,-2.653762
6928,0.6776557397\c,-3.3996979563,-0.586007303,0.896743874\c,-3.550328
2416,-2.3401360458,2.7177301469\c,-3.8779023541,-0.5162188361,-0.41505
34237\c,-4.3226549462,0.6913974675,-0.9563779389\c,-4.2930565241,1.854
2413707,-0.1894252275\c,-3.825991489,1.7975530261,1.1241299615\c,-3.38
79538247,0.5882102848,1.6602487126\H,-3.8842647462,-1.4173053542,-1.02
52286922\H,-4.6861619228,0.7228034245,-1.9800283783\H,-4.626181937,2.7
980260348,-0.6114689947\H,-3.7970719591,2.6985013375,1.7309266576\H,-3
.016432813,0.5639157179,2.6836010962\H,-3.1478386461,-3.2977703504,3.0
648954764\H,-4.6225891528,-2.4611932406,2.5368457868\H,-3.4253050341,-
1.6118991759,3.5269419614\H,3.3200797026,1.8351213735,-0.8736217809\H,
2.028026034,1.9620405359,0.8278003719\H,0.603527245,3.7354449437,2.189
4240589\H,-0.7724235707,3.0883576848,3.0964091308\H,-0.938304998,3.440
2659113,1.3672787001\H,1.8346014613,1.745979683,3.2549666612\H,1.34096
72825,0.0768434739,2.8956064316\H,0.3395026963,1.0999469338,3.94390748
1\c,-0.7474616695,2.1409179262,-1.1529197375\c,-1.3053873345,3.0018390
291,-2.0869224682\c,-0.6402232063,4.1809384075,-2.4371827724\c,0.58004
58947,4.4933780077,-1.8359013799\c,1.1240886334,3.6253624848,-0.892506
0884\H,-1.287943514,1.2389416198,-0.8813481998\H,-2.2610652967,2.77646
06973,-2.5513012627\c,-1.2726296223,5.0703660498,-3.4434416777\H,1.095
5775198,5.4095172716,-2.1046358618\H,2.0705702996,3.8776802596,-0.4186
438133\o,-0.5394198187,6.1720825169,-3.7135510503\o,-2.3346142917,4.86
11344914,-3.9841136988\H,-1.0347923539,6.6829029321,-4.3764543842\\Ver
sion=ES64L-G09Revd.01\HF=-1484.589671\RMSD=8.418e-09\RMSF=1.209e-06\Di pole=0.4966011,-0.2327637,0.4451943\Quadrupole=-6.2229545,7.4611301,-
1.2381756,4.4187185,-3.0307035,1.6436841\PG=C01 [X(C31H39N1O3)]\\@
```

7- (core)

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1\1\GINC-R117\FOpt\UM062X\Gen\C9H9N1O3(1-,2)\ROOT\02-Sep-2013\0\\#M062
X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdisk=
1610612736\tnca1_r+core.freq\1,2\c,2.5167728888,-0.9710647982,0.387
5794071\N,1.5848241524,-1.0042441096,-0.7298163587\o,1.3201017911,0.09
70843697,-1.317560468\c,0.6055621127,-2.0993822608,-0.7905329494\H,1.1
443087427,-3.0238129238,-1.0366288923\c,-0.1457172717,-2.2717292475,0.
5090028122\H,-0.0519352434,-1.839821474,-1.6236411093\H,3.3437171319,-
0.3154467545,0.1110572562\c,-0.9812743877,-1.2522671461,0.980465536\c,
-1.63530512,-1.389941444,2.2024566109\c,-1.4733992107,-2.5427988515,2.
```

9781877541\c,-0.640472022,-3.5567215392,2.504684782\c,0.0213638999,-3.  
 4217504291,1.2835685435\c,-2.2023724375,-2.6915826305,4.3408101221\o,-  
 1.9764253114,-3.7628654463,4.945886145\o,-2.9225937731,-1.7213928578,4  
 .6628092167\h,2.0194465925,-0.5907566891,1.2880039826\h,2.8780274497,-  
 1.9834580229,0.5877925197\h,-1.1036446102,-0.3481776903,0.3844405707\h  
 ,-2.2887122813,-0.6139913198,2.5915906991\h,-0.5284190529,-4.443060044  
 6,3.1230059106\h,0.6753709602,-4.21709969,0.9244659093\\Version=ES64L-  
 G09RevD.01\HF=-628.5627205\\$2=0.755405\\$2-1=0.\\$2A=0.750017\RMSD=6.991  
 e-09\RMSF=3.123e-06\Di pole=3.3436948,0.1455962,-4.1042552\Quadrupole=2  
 1.6767827,15.1436946,-36.8204773,-22.8712595,40.8691977,43.7221902\PG=  
 C01 [X(C9H9N1O3)]\\@

7-

1\\1\GINC-D20\FOpt\UM062X\Gen\C15H21N1O3(1-,2)\ETS502\01-Sep-2013\0\\#M  
 062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdi-  
 sk=2147483648\\tnca1\_r+.freq\\-1,2\N,1.5183359703,-0.9421231352,-0.675  
 7649406\o,1.0162653061,0.176984436,-1.0269170277\c,3.7234632336,0.0491  
 376419,-0.5078157577\c,-0.2554233574,-2.0717487278,-1.9699877906\c,2.7  
 249838542,-0.8732369173,0.1979910511\c,0.6356387525,-2.1333767128,-0.7  
 17809713\c,2.3355787405,-0.2868423077,1.5619699381\c,-0.1395350148,-2.  
 2823882668,0.5777946842\c,3.3419721433,-2.260630003,0.3712017964\h,2.6  
 845780872,-2.9318982237,0.931143479\h,4.2734341741,-2.1583712628,0.937  
 8988736\h,3.2401712568,-0.1024382942,2.153283601\h,1.6845416046,-0.966  
 5749212,2.1189603304\h,1.8074880644,0.6607056082,1.4193405069\h,3.9833  
 112627,-0.3511555048,-1.4945872947\c,-1.150511709,-3.3107339045,-2.028  
 060701\h,3.2958701298,1.0451678871,-0.6399494135\c,0.5929173866,-1.959  
 2417381,-3.2380456109\h,4.6368238996,0.1275518476,0.0914572824\h,-0.88  
 53528822,-1.1791467128,-1.8837838912\h,3.582262489,-2.713871717,-0.597  
 8760054\h,1.2925694701,-3.0048610179,-0.8309831741\h,-0.5450755255,-4.  
 2267675048,-2.0649881258\h,-1.7735921625,-3.2855496166,-2.9290777927\h  
 ,-1.8058715667,-3.377493282,-1.1554176569\h,1.2708688672,-2.8202697749  
 ,-3.3217757679\h,1.1914187065,-1.0446481634,-3.2378288061\h,-0.0461102  
 067,-1.9530510273,-4.1285194096\c,-0.9577184215,-1.2482134114,1.046725  
 9123\c,-1.6582137963,-1.3959384933,2.2424313707\c,-1.5625170941,-2.571  
 5616657,2.9940290674\c,-0.7516212647,-3.6030757784,2.519286622\c,-0.04  
 63215845,-3.460070885,1.3237097758\h,-1.0196872251,-0.3201908964,0.479  
 9021116\h,-2.2945734161,-0.6055283256,2.6309375952\c,-2.3393823977,-2.  
 7285512097,4.3285768038\h,-0.6920251223,-4.5093694984,3.1157141998\h,0  
 .5841088635,-4.2732897995,0.9605926222\o,-3.0377895241,-1.7431115788,4  
 .6523880281\o,-2.1687349913,-3.8214251423,4.9131142276\\Version=EM64L-  
 G09RevC.01\HF=-864.3404169\\$2=0.754795\\$2-1=0.\\$2A=0.750015\RMSD=5.420  
 e-09\RMSF=2.211e-06\Di pole=4.7395776,0.6038095,-5.8094652\Quadrupole=2  
 0.4832254,14.4582881,-34.9415136,-23.9248173,42.3608462,42.7142515\PG=  
 C01 [X(C15H21N1O3)]\\@

7^-P (core)

1\\1\GINC-R101\FOpt\RM062X\Gen\C13H16N1O3(1-)\ROOT\08-Oct-2013\0\\#M062  
 X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdisk=2147483648\\pstnca1core.freq\\-1,1\o,0.5820306342,-0.6727405463,0.9053  
 555374\N,0.477371725,0.2464626628,-0.1837966924\c,1.7464058738,0.19238  
 71395,-0.8922361657\c,0.2393958079,1.5612690077,0.4275173771\c,0.07018  
 26843,2.6320966742,-0.6209646901\c,-0.999302478,2.5779399437,-1.522295  
 8637\c,-1.1478480339,3.5555940911,-2.5030927936\c,-0.2358652935,4.6106  
 145602,-2.6085412324\c,0.8296998215,4.6634318897,-1.7095169476\c,0.983  
 6389551,3.6835410422,-0.7274018891\c,-0.4720261909,-1.6269432786,0.820  
 5917466\c,-0.2360770543,-2.5867460916,-0.3147411882\c,-1.0072068304,-2  
 .6658186009,-1.3966372157\c,-0.4056817963,5.6987117771,-3.7019012736\o  
 ,-1.3981739964,5.5483526807,-4.4487618757\c,-0.4976993952,-2.338462974  
 7,2.1658380758\o,0.4710275376,6.5913211443,-3.7015866633\h,2.593647454  
 ,0.4458841638,-0.2336198369\h,-0.6706332628,1.4561966301,1.0301756176\h,  
 1.8821372383,-0.8167956722,-1.2883357566\h,1.7047083245,0.9050237676  
 ,-1.7190181809\h,-0.6565510265,-1.6162150229,2.9716681232\h,-1.2992777  
 686,-3.0830023614,2.1860451788\h,0.4564158407,-2.8471288837,2.34121164  
 16\h,-1.4166506495,-1.0906166516,0.6505146179\h,-0.7995468937,-3.36669  
 26698,-2.2003969584\h,0.6433451255,-3.2259074615,-0.2120390573\h,-1.86  
 45315892,-2.0082413962,-1.5214970559\h,1.0677999671,1.8167208429,1.110  
 6628363\h,-1.7077690356,1.7531516488,-1.4513768347\h,-1.970245628,3.53  
 35300043,-3.2128721709\h,1.5280224772,5.4900415766,-1.8076447708\h,1.8  
 229264561,3.731124364,-0.0334576392\\Version=ES64L-G09RevD.01\HF=-785.  
 1221683\RMSD=8.639e-09\RMSF=8.437e-06\Di pole=0.5745846,-7.0581782,4.57  
 32795\Quadrupole=57.056241,-61.7537077,4.6974666,8.0429394,-8.3405513,  
 80.4712098\PG=C01 [X(C13H16N1O3)]\\@

7^-P

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1\1\GINC-R147\FOpt\RM062X\Gen\C31H38N1O3(1-)\ROOT\06-Oct-2013\0\\#M062
X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdisk=
3489660928\pstnca1.2.freq\~-1,1\N,1.2420245323,0.1348781739,0.0145913
154\O,0.7379106861,-0.8477692843,0.9201149886\C,-0.5688864861,-1.24523
53798,0.4977095378\C,-1.3201532051,-1.7438328003,1.7281304524\C,-0.528
7885744,-2.2302718088,-0.6531025913\C,3.5436760659,-0.2478531554,0.958
2554012\C,0.2141679526,1.6204247923,1.8388851334\C,2.649790861,-0.2215
499767,-0.2923051296\C,1.0465760045,1.5331910141,0.5342500541\C,2.6710
552543,-1.6075466017,-0.9438551973\C,0.4610274878,2.405092964,-0.56643
70756\C,3.1776262668,0.7925454049,-1.3136991065\H,2.4823584538,0.88524
12623,-2.1539383728\H,4.1471080008,0.4473087261,-1.689743859\H,3.69423
45959,-1.84529535,-1.2569094219\H,2.0200005861,-1.6302913263,-1.823784
714\H,2.335092994,-2.3785181796,-0.2466477698\H,4.5672450164,-0.523899
7554,0.6789277764\C,-0.231548226,3.0618154802,2.1097836558\H,3.5853495
414,0.7272215588,1.4550043936\C,1.0008776707,1.1093674006,3.0501960683
\H,3.1711485423,-0.9858684357,1.6758896686\H,-0.6943452833,1.020147367
7,1.7134715839\H,-1.1599612113,-1.0152999507,2.5346009181\C,-2.8319037
959,-1.890728876,1.4624478045\H,-0.9111561483,-2.6992378816,2.08093139
44\H,-1.077731546,-0.3495410117,0.1405883816\C,-0.8141436502,-1.786045
742,-1.9464939018\C,-0.7339422479,-2.6580660433,-3.0324504907\C,-0.363
9678579,-3.9869061543,-2.8338435698\C,-0.0773688182,-4.4399734985,-1.5
450121117\C,-0.1626505139,-3.5660480848,-0.4638095839\H,-1.077323295,-
0.7421439771,-2.103280273\H,-0.9506210153,-2.293899707,-4.0327778419\H
,-0.2958583548,-4.6671944329,-3.6784826836\H,0.2169004726,-5.473864976
8,-1.3844587646\H,0.0828154912,-3.9219914297,0.5345184412\H,-2.9648804
343,-2.6667080505,0.6959240775\C,-3.3988271302,-0.5969915203,0.9013994
341\C,-3.5582414087,-2.3441567538,2.732419559\C,-3.8412070835,-0.52787
92983,-0.4228789104\C,-4.2473059247,0.6839211979,-0.9845052241\C,-4.21
72628876,1.8517751846,-0.2258839456\C,-3.7943860424,1.79339786,1.10210
24816\C,-3.3930675168,0.5805500451,1.6591444582\H,-3.8323915499,-1.430
0896929,-1.0319655388\H,-4.5583269295,0.7224493996,-2.024826887\H,-4.4
884304346,2.8024697988,-0.6751425635\H,-3.7509499817,2.7012161582,1.69
76094484\H,-3.0380824731,0.5598728731,2.6887207189\H,-3.1533769586,-3.
2978971077,3.0897838377\H,-4.6297227666,-2.4696798978,2.5473112265\H,-
3.4398715632,-1.6086047122,3.5362134622\H,3.3219066006,1.7883650861,-0
.8866075159\H,2.0271578437,1.9599160876,0.7969687696\H,0.6333687326,3.
7362063071,2.1597825917\H,-0.7521066596,3.1098325778,3.074406845\H,-0.
9007003639,3.4394407841,1.3326145687\H,1.8703625534,1.7570617696,3.229
6041961\H,1.3534641409,0.086017716,2.9124567981\H,0.3766623051,1.14334
88264,3.9522001015\C,-0.7801769,2.1149398749,-1.1443373348\C,-1.360648
4941,2.9809181689,-2.0666064075\C,-0.7199170753,4.1628647528,-2.447652
4253\C,0.5205497692,4.4529658576,-1.8794669126\C,1.0996336787,3.587002
3113,-0.9490106909\H,-1.3232745512,1.2198833206,-0.8487204215\H,-2.330
2952608,2.7702047945,-2.5104452914\C,-1.3861655646,5.1302583293,-3.459
3206791\H,1.0100057377,5.3744370644,-2.1832100538\H,2.062399102,3.8393
334786,-0.5019888365\O,-0.7115119207,6.1419792962,-3.7512856093\O,-2.5
218578351,4.7809117881,-3.8551888375\Version=ES64L-G09RevD.01\HF=-148
4.0447298\RMSD=9.110e-09\RMSF=3.672e-06\Dipole=1.3178574,-7.6927796,5.
2239467\Quadrupole=36.1419136,-42.8913391,6.7494255,24.7479407,-18.284
4883,67.1040189\PG=C01 [X(C31H38N1O3)]\@
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17 (core)

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1\1\GINC-X132\FOpt\UM062X\Gen\C4H8N1O3(2)\GXG501\25-Jan-2013\0\\#M062X
/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=53687091
2\tn_rcore+.freq\0,2\O,0.7640660454,0.2477356769,-0.5770965629\N,1.4
239165197,-0.8391431895,-0.5083934983\C,0.7671974509,-2.1004035124,-0.
806700085\C,2.7093018219,-0.8059398319,0.1808908816\H,3.081681956,-1.8
301648654,0.2592971945\C,3.6889301264,0.0665332592,-0.5900575178\C,4.0
647181985,-0.5739776451,-1.9033105734\O,4.8217954751,0.2383959576,-2.6
618196771\H,2.5531326827,-0.3994748518,1.1867341085\H,-0.0416567806,-1
.8867032228,-1.5052407364\H,0.3519871193,-2.5487833176,0.1056458633\O,
3.7503846486,-1.686681007,-2.2543047318\H,3.2413929927,1.0461794277,-0
.7872576825\H,4.6064866945,0.2394429383,-0.016306592\H,1.490233362,-2.
7816373418,-1.2614905482\H,5.0280286869,-0.2378754742,-3.4856758426\V
ersion=EM64L-G09RevB.01\State=2-A\HF=-437.4329853\S2=0.75513\S2-1=0.\S
2A=0.750016\RMSD=7.416e-09\RMSF=7.994e-06\Dipole=0.8759475,-0.5952816,
0.2522324\Quadrupole=-1.1975363,-2.773573,3.9711092,4.83755,-0.4134779
,-1.80369\PG=C01 [X(C4H8N1O3)]\@
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17

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1\1\GINC-X149\FOpt\UM062X\Gen\C15H22N1O3(2)\GXG501\25-Jan-2013\0\\#M06
2X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=536870
```

```

912\\tn_r+.freq\\0,2\\N,1.4998782705,-0.9410015638,-0.6280711153\\O,0.98
31255048,0.1796792207,-0.948833724\\C,3.7278988482,0.0123083061,-0.5893
898365\\C,-0.2650249891,-2.0781732738,-1.9390809488\\C,2.7452688645,-0.8
757938831,0.1856011626\\C,0.649813796,-2.1443914124,-0.7021152236\\C,2.4
221790723,-0.1925693233,1.5230236508\\C,-0.1262681421,-2.3177456713,0.5
935842349\\C,3.3327107605,-2.263591904,0.446112489\\H,2.665876684,-2.859
1301376,1.0770873635\\H,4.2738332369,-2.1397774663,0.9924310274\\H,3.344
8023112,-0.0223313754,2.0885686232\\H,1.7583796956,-0.8210304258,2.1245
948556\\H,1.9312477194,0.7684668983,1.3458435878\\C,4.0803700471,-0.4853
63336,-1.9700632742\\C,-1.1218725994,-3.344105147,-2.0147609277\\H,3.308
2023344,1.0170594518,-0.7018241756\\C,0.5537921396,-1.9051101025,-3.218
4356186\\H,4.660998174,0.1183481744,-0.0230533103\\H,-0.922008908,-1.208
8374084,-1.8169634259\\H,3.5410437655,-2.8027269862,-0.4798267641\\H,1.3
238855743,-2.9984030102,-0.8334810516\\H,-0.4893165169,-4.2391106922,-2
.0836260207\\H,-1.752866676,-3.3159409265,-2.9087918229\\H,-1.7735159071
,-3.4558109396,-1.1430682885\\H,1.27506199,-2.7236248315,-3.332348843\\H
,1.1113046056,-0.9662705541,-3.2139790429\\H,-0.1089303772,-1.910823149
3,-4.0905494314\\C,-0.9137475011,-1.2717403497,1.086861924\\C,-1.6348137
956,-1.4311686595,2.2672380605\\C,-1.5813087378,-2.6379398876,2.9671071
569\\C,-0.8025941853,-3.6847685923,2.4789966504\\C,-0.0782640397,-3.5217
726011,1.2976438252\\H,-0.940458264,-0.3275119927,0.5472744969\\H,-2.239
3117877,-0.6110781492,2.6441876103\\H,-2.143936082,-2.7598875067,3.8880
388152\\H,-0.7564840548,-4.6277673103,3.0161996646\\H,0.5284247748,-4.34
12961633,0.9158424114\\O,3.7295931979,-1.5207430549,-2.4827292224\\O,4.8
78570638,0.3946529,-2.6088594151\\H,5.0676905588,0.0251958367,-3.489507
1275\\Version=EM64L-G09RevB.01\\State=2-A\\HF=-864.8780298\\S2=0.754892\\S
2-1=0.\\S2A=0.750016\\RMSD=3.731e-09\\RMSF=6.576e-06\\Dipole=0.5259801,-0.
4314567,0.636401\\Quadrupole=2.1285454,-3.6962445,1.5676991,1.4153307,-
3.1529302,-1.0977238\\PG=C01 [X(C15H22N1O3)]\\@
```

**17-P (core)**

```

1\\1\\GINC-V1446\\FOpt\\RM062X\\Gen\\C8H15N1O3\\GXG501\\14-Jan-2013\\0\\#M062X/
gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=671088640
\\dtn_core.freq\\0,1\\N,1.332539283,-0.3598562563,-0.062286655\\O,1.0944
039329,0.7361782402,-0.9395259523\\C,0.2820820072,-0.3614517805,0.95050
669\\C,2.6679399975,-0.1515965066,0.4841230334\\H,0.5162078386,-1.178382
6276,1.6419695734\\H,-0.6540865697,-0.6086715097,0.4457861395\\C,0.12496
77584,0.9640258597,1.7231378284\\H,0.970939038,1.1508668541,2.387054010
3\\H,0.0435878291,1.7796788438,0.9968699811\\C,-1.116347647,0.9323428255
,2.5700541561\\O,-1.1571051159,0.8912096732,3.7755483821\\O,-2.237570334
5,0.9265135637,1.8126270128\\H,-2.9964541762,0.8846981292,2.4205008575\\
H,2.7870987864,0.8347938381,0.9538015151\\H,3.3939775171,-0.2407975586,
-0.3277741252\\H,2.8655749156,-0.9366675707,1.2194630018\\C,0.9817569075
,0.2806798725,-2.2846811559\\H,1.6893568267,-0.5477116027,-2.4202886663
\\C,-0.4127184349,-0.1927983241,-2.6213037885\\C,1.38232383,1.4567849997
,-3.1695974837\\H,0.7255886232,2.3082558426,-2.9668741368\\H,2.417629686
7,1.7488566903,-2.9719904289\\H,1.2823681559,1.1905536352,-4.2262464744
\\H,-0.4867647002,-0.8367862248,-3.4977593005\\C,-1.5155758102,0.1738372
421,-1.9717995267\\H,-1.4725255907,0.8259205804,-1.1026570961\\H,-2.4964
255546,-0.1665047287,-2.2893563914\\Version=EM64L-G09RevB.01\\State=1-A
\\HF=-593.9901218\\RMSD=7.173e-09\\RMSF=4.076e-06\\Dipole=0.1827064,-0.202
205,-0.7433453\\Quadrupole=6.968806,-0.9117668,-6.0570391,-0.367827,-0.
2977408,-0.2915556\\PG=C01 [X(C8H15N1O3)]\\@
```

**17-P**

```

1\\1\\GINC-V1427\\Freq\\RM062X\\Gen\\C31H39N1O3\\GXG501\\12-Feb-2013\\0\\#M062X
/gen 6D SCF=Tight INT(grid=ultrafine) IOP(2/17=4) Freq=Noramam maxdisk
=2013265920\\dtn.freq\\0,1\\N,1.2322813018,0.1681536219,-0.0043352681\\O
,0.7368855049,-0.827641022,0.8823933186\\C,-0.5690690346,-1.24638666,0.
4687422334\\C,-1.3045991534,-1.7329988316,1.7139632744\\C,-0.5259378901,
-2.2586466958,-0.6559031659\\C,3.5033372258,-0.2568488214,0.9390724453\\
C,0.1958864011,1.6205988671,1.8412736344\\C,2.6307959761,-0.1869696492,
-0.3493018109\\C,1.0496022203,1.55013643,0.549922432\\C,2.6367154562,-1.
5521936222,-1.0407969356\\C,0.4848700877,2.4481162778,-0.5426757939\\C,3
.1608385476,0.8602051926,-1.3338599617\\H,2.4492524498,0.9829844186,-2.
1565267699\\H,4.1213245053,0.5313310352,-1.7373722447\\H,3.6385898213,-1
.7649991724,-1.4290148766\\H,1.9322777984,-1.5526271683,-1.8782036383\\H
,2.360765405,-2.3525486326,-0.3515619426\\C,4.9089773022,-0.7103218798,
0.653327746\\C,-0.2516686141,3.0581048885,2.1313124316\\H,3.5766418275,0
.7333692069,1.3991092222\\C,0.9666704407,1.0890186535,3.0534996449\\H,3.
0315512353,-0.9492996411,1.6397486578\\H,-0.709715506,1.0222698727,1.69
06542061\\H,-1.144482307,-0.9972026853,2.5134681363\\C,-2.8158876332,-1.
```

8979626855, 1.4626801583\H, -0.8840985479, -2.6812625393, 2.0700175308\H, -  
 1.0882803186, -0.3614099351, 0.0966833829\C, -0.9015022891, -1.8792977036,  
 -1.945870537\C, -0.8280108753, -2.7844153859, -3.0052179547\C, -0.37377521  
 2, -4.0821139822, -2.7806602706\C, 0.0022099158, -4.471194692, -1.493699994  
 \C, -0.0777457454, -3.5652100547, -0.4397029816\H, -1.2370967878, -0.859435  
 8248, -2.1228146272\H, -1.1172160056, -2.4729493605, -4.0049419519\H, -0.31  
 03236388, -4.7883771628, -3.6034565656\H, 0.361371167, -5.4805715107, -1.31  
 40679555\H, 0.2378323792, -3.8702337227, 0.5556496356\H, -2.9477626261, -2.  
 6759895906, 0.6985578104\C, -3.4026961785, -0.6110828187, 0.9079836295\C, -  
 3.5267209417, -2.3557024933, 2.7400410856\C, -3.8949027525, -0.5551914305,  
 -0.3990170629\C, -4.3530516455, 0.6453335342, -0.9448525917\C, -4.32191748  
 39, 1.8143305662, -0.1876877387\C, -3.8405175254, 1.7715922679, 1.121169709  
 7\C, -3.3904600199, 0.569179608, 1.6621805884\H, -3.9014618481, -1.46105684  
 68, -1.0019818114\H, -4.7284543003, 0.6649996768, -1.964534964\H, -4.665585  
 2564, 2.7531363081, -0.6122821152\H, -3.8088120281, 2.6779874513, 1.7195160  
 261\H, -3.0078662747, 0.555345125, 2.6816204553\H, -3.1116131264, -3.306346  
 1076, 3.0914534058\H, -4.5984566977, -2.4900365101, 2.5654736865\H, -3.4057  
 355597, -1.6205141919, 3.5435600604\H, 3.3261730415, 1.8350486887, -0.86822  
 70688\H, 2.0284190845, 1.9677835981, 0.8310621789\H, 0.6112261004, 3.733439  
 7437, 2.1984435012\H, -0.7749961344, 3.0906124513, 3.0936416957\H, -0.92410  
 71726, 3.4482857145, 1.3626430695\H, 1.8406704048, 1.724841147, 3.249743393  
 4\H, 1.3069311814, 0.0626454527, 2.9103251361\H, 0.3339484389, 1.1199352773  
 , 3.948399372\C, -0.7352463224, 2.1600085829, -1.1627754873\C, -1.281849575  
 9, 3.0296544673, -2.1020404006\C, -0.6115928278, 4.2042245517, -  
 2.4470423457\C, 0.6025414338, 4.5038090333, -  
 1.8342997204\C, 1.1399964862, 3.630982529 2, -0.8877710363\H, -  
 1.2832624118, 1.2598600374, -0.896696075\H, -2.2368243 376, 2.7882041314, -  
 2.5616541155\H, -1.0343888744, 4.8799065981, -3.1848593  
 664\H, 1.1340794301, 5.4156542176, -2.0913603154\H, 2.0861788861, 3.8764723  
 598, -0.408471013\O, 5.7857726277, -0.027251238, 0.1774305644\O, 5.11070507  
 04, -2.0076521212, 0.9718820668\H, 6.0320123265, -2.2187001941, 0.738160948  
 5\\Version=EM64L-G09RevB.01\\State=1-A\\HF=-1484.5823776\\RMSD=9.639e-10\\  
 RMSF=5.066e-06\\ZeroPoint=0.6457084\\Thermal=0.6794188\\Dipole=-0.8147044  
 , -0.3868727, 0.0333629\\ PG=C01 [X(C31H39N1O3)]\\@

**17-** (core)

1\\1\\GINC-V1435\\FOpt\\UM062X\\Gen\\C4H7N1O3(1-,2)\\GXG501\\09-Mar-2013\\0\\#M  
 062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdi  
 sk=671088640\\tnc\_rcore+.freq\\-1,2\N,3.7349501946,0.1958494814,-0.761  
 7331591\C,2.8890194784,0.4389805354,-1.9209029248\C,3.1913809417,-0.12  
 88275396,0.5647352797\O,4.938441843,0.617858388,-0.8078414468\H,3.5192  
 668562,0.309183209,-2.8023736906\H,2.0497307703,-0.2606857283,-1.94219  
 88318\H,2.5089650737,1.4717805694,-1.9031210595\H,3.7701363919,-0.9775  
 422236,0.9429811444\H,3.390781291,0.7464197097,1.2002587218\C,1.715856  
 1905,-0.495765757,0.5528316705\H,1.1040957045,0.3092931596,0.129812521  
 4\H,1.4132071376,-0.6275336743,1.5993752679\C,1.4318248551,-1.84438855  
 23,-0.1864908231\O,0.5305908989,-1.8076929587,-1.0585204178\O,2.145562  
 3724,-2.8028116186,0.1820887479\\Version=EM64L-G09RevB.01\\HF=-436.8873  
 442\\S2=0.755239\\S2-1=0.\\S2A=0.750018\\RMSD=9.004e-09\\RMSF=1.016e-06\\Dip  
 ole=0.5142236,2.3475229,0.2996185\\Quadrupole=-16.6500732,-1.9332241,18  
 .5832973,6.7480123,3.2509578,-2.4755868\\PG=C01 [X(C4H7N1O3)]\\@

**17-**

1\\1\\GINC-V1404\\FOpt\\UM062X\\Gen\\C15H21N1O3(1-,2)\\GXG501\\10-Mar-2013\\0\\  
 #M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm max  
 disk=671088640\\tnc\_r+.freq\\-1,2\N,3.6708262858,0.0565785784,-0.80892  
 34783\O,2.9187075296,0.3501677454,-1.7981650299\C,4.0270472267,-0.5271  
 492924,1.5967475237\C,5.6923511925,0.802748017,-2.0105459617\C,2.99969  
 49761,-0.3252537207,0.4691575033\C,5.0739756668,-0.2790950673,-1.10588  
 17632\C,1.9995451508,0.7840883032,0.8041377641\C,5.1799813263,-1.68297  
 61439,-1.6743284433\C,2.2501331705,-1.644052711,0.2138744972\H,1.55444  
 79695,-1.5215719121,-0.6231872069\H,1.684267862,-1.9257383252,1.109408  
 551\H,1.4725463303,0.5197516869,1.7277887513\H,1.275050064,0.892799049  
 2,-0.0077600075\H,2.5278951892,1.7233818977,0.9794588845\C,4.986069233  
 9,0.6713245231,1.9049993445\C,7.1793863717,0.5003876797,-2.2100156218\  
 H,3.4414782883,-0.7224882445,2.5041659671\C,5.50991363,2.1791521632,-1  
 .3655571809\H,4.6218204261,-1.426031438,1.3929327993\H,5.1796953967,0.  
 7804970618,-2.9817672392\H,2.9486621827,-2.454111748,-0.0250689193\H,5  
 .6236729764,-0.2434489957,-0.1614896066\H,7.6899119926,0.4801936768,-1  
 .23870954\H,7.6471258056,1.2793267027,-2.8234440963\H,7.3409421148,-0.  
 464185046,-2.7039543396\H,5.9194585743,2.178872186,-0.3474825601\H,4.4  
 523075907,2.4494812373,-1.3031569395\H,6.0293087302,2.9454250459,-1.95

46348365\c, 4.4636037838, -2.0720240341, -2.8122459978\c, 4.580075682, -3.3  
 685628372, -3.3092808157\c, 5.4170714773, -4.2926396892, -2.6808376859\c, 6  
 .1350632554, -3.9111330412, -1.5485079214\c, 6.0139387472, -2.6141468853, -  
 1.0487361726\h, 3.7995059319, -1.3530319389, -3.2851740251\h, 4.0129741754  
 , -3.6614798415, -4.1895800997\h, 5.5054751802, -5.3037406089, -3.070308591  
 5\h, 6.7868507532, -4.6240545352, -1.0497749639\h, 6.5645783609, -2.3098528  
 937, -0.1599556501\o, 4.4399876036, 1.7200537506, 2.3080078183\o, 6.2097597  
 947, 0.4459006451, 1.7136442898\version=EM64L-G09RevB.01\HF=-864.339286  
 1\s2=0.754945\s2-1=0.\s2a=0.750016\rmsd=7.305e-09\rmsf=6.773e-06\dipol  
 e=-0.4588784, -2.9122538, -2.8697011\quadrupole=-54.5877283, 31.7933877, 2  
 2.7943405, -15.8467652, -19.2038574, -9.6217544\pg=c01 [x(c15h21n103)]\\@

### 17<sup>-</sup>P (core)

dtnc\_core 1\1\GINC-V1404\FOpt\RM062X\Gen\C8H14N1O3(1-)\GXG501\09-Mar-  
 2013\0\#M0 62X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)  
 Nosymm maxdis k=671088640\dtnc\_core.freq\~-1,1\N,1.2282347409,-  
 0.3517836,0.73551569 21\c,0.6543408196,0.2953001419,-  
 0.4642999105\c,0.7227433394,0.21783045 8,1.9724697276\o,2.6260860782,-  
 0.0371332792,0.7463503073\c,3.352979014 5,-  
 1.0463051682,0.0472375952\h,2.7220851207,-1.4058388666,-0.774711920  
 7\c,3.672154385,-2.2030123882,0.9851861659\c,4.5834628049,-0.391296964  
 3,-0.5396212071\h,4.3135137571,-1.855057228,1.803577235\h,2.7431899745  
 ,-2.5972479816,1.4084269616\h,4.1902467781,-3.0093809191,0.4525359031\h,  
 5.5450356946,-0.6480349315,-0.0908301034\c,4.5046938369,0.4880127451  
 ,-1.5391856264\h,3.5477926175,0.7810797251,-1.9861482678\h,5.402273414  
 6,0.9662286477,-1.926697333\h,0.9620882631,1.2869188728,2.0717175675\h  
 ,1.1566799693,-0.3258651629,2.8170822401\h,-0.3647127453,0.0928969555,  
 1.9816893986\h,-0.4030629445,0.0000620772,-0.4829377477\h,1.133470756,  
 -0.1641037873,-1.3341786416\c,0.8174019579,1.8076803771,-0.59007141\h,  
 1.7857250158,2.0876114668,-0.1536313705\h,0.0285935472,2.3590297527,-0  
 0.678464538\c,0.86402768,2.2537788472,-2.0878064901\o,0.1683078637,3.2  
 436185416,-2.3965199836\o,1.6315852603,1.5682096682,-2.8150313278\ver  
 sion=EM64L-G09RevB.01\HF=-593.4399249\rmsd=2.817e-09\rmsf=4.755e-06\dipole  
 =1.5095767,-3.0147925,3.3314288\quadrupole=9.9220004,-4.3941266,-5  
 .5278739,-2.7428907,5.8735099,21.2612599\pg=c01 [x(c8h14n103)]\\@

### 17<sup>-</sup>P

1\1\GINC-V1437\Freq\RM062X\Gen\C31H38N1O3(1-)\GXG501\16-Apr-2013\0\#M  
 062X/gen 6D SCF=Tight INT(grid=ultrafine) Freq=Noramian IOP(2/17=4) max  
 disk=1879048192\dtnc.freq\~-1,1\N,1.2110323407,-0.3510255539,-0.01722  
 83317\o,0.8181195059,0.6832061412,-0.922608404\c,-0.3699166969,1.30720  
 60367,-0.4590487648\c,-1.0806554003,1.8851297541,-1.6827402522\c,-0.12  
 11575457,2.336608632,0.6249950426\c,3.5086937889,-0.3559201493,-1.0858  
 485478\c,-0.114850998,-1.6634647559,-1.786130142\c,2.6932150534,-0.223  
 6084859,0.2159803404\c,0.7919482069,-1.6939471156,-0.5290602224\c,2.95  
 18601697,1.1487016494,0.8413211033\c,0.1269770731,-2.4699406997,0.6016  
 253832\c,3.0714161684,-1.2953710762,1.2441097551\h,2.413955034,-1.2293  
 555441,2.1201209244\h,4.1139517992,-1.1427841811,1.5291710974\h,3.9970  
 833445,1.2008805297,1.1585125991\h,2.2978703564,1.3079340393,1.7073286  
 215\h,2.7934959653,1.9482867381,0.1147199518\c,5.0254841523,-0.0405608  
 21,-0.8739314817\c,-0.7950106809,-3.0180192714,-2.0221415221\h,3.42665  
 22391,-1.3779130179,-1.4795966553\c,0.6797391816,-1.2854958166,-3.0394  
 778865\h,3.1059138339,0.3477274632,-1.8206341428\h,-0.9096016748,-0.92  
 65075399,-1.6207713414\h,-1.069513444,1.1213138726,-2.4719331213\c,-2.  
 533417529,2.2934930899,-1.3773433856\h,-0.5297501898,2.7490497961,-2.0  
 741681475\h,-1.0116916107,0.5323258748,-0.0328857375\c,-0.57240488,2.1  
 071058092,1.9251213654\c,-0.3300083985,3.0348160036,2.9390521096\c,0.3  
 74031848,4.2032520231,2.6578593665\c,0.8350045665,4.4381390036,1.36101  
 52582\c,0.5850541266,3.5120092998,0.3529552574\h,-1.0955400933,1.17934  
 6684,2.1483709468\h,-0.6757273605,2.8354486596,3.9498796682\h,0.577120  
 482,4.9222656657,3.446898767\h,1.4055249666,5.3360258981,1.1403959898\h,  
 0.9810069475,3.6808779104,-0.6459285914\h,-2.508499544,3.0884828023,  
 -0.6194316055\c,-3.3017636597,1.1247260431,-0.7848464001\c,-3.21416182  
 27,2.8485140555,-2.6328713148\c,-3.7727549961,1.169594061,0.5302512528  
 \c,-4.3962784704,0.0633990671,1.1102576466\c,-4.556540902,-1.111773854  
 2,0.3795783238\c,-4.0999651573,-1.1676631736,-0.9375613922\c,-3.484821  
 7828,-0.0581229982,-1.5125769157\h,-3.6212358011,2.074638189,1.1151643  
 561\h,-4.7419460792,0.1179132935,2.1393899938\h,-5.0196437818,-1.98289  
 25983,0.8343622242\h,-4.2060296037,-2.0834998673,-1.5126814997\h,-3.11  
 4093342,-0.1259555526,-2.5340332929\h,-2.6630079264,3.7138609229,-3.01  
 66382853\h,-4.2425457086,3.158185502,-2.4199628405\h,-3.2463374686,2.0  
 940703066,-3.4273284078\h,3.0145004234,-2.3079897925,0.8336521363\h,1.

```

6834367447,-2.2622288614,-0.8295988245\H,-0.0506625588,-3.8217598105,-
2.0968283478\H,-1.3498507849,-2.9895430769,-2.9681249861\H,-1.49334784
77,-3.2817480311,-1.2223056025\H,1.4258856509,-2.0610084746,-3.2565672
365\H,1.203299457,-0.3365714547,-2.9226413234\H,0.0091685829,-1.216730
6709,-3.9062439572\C,-1.0128990213,-1.9841088157,1.2514711656\C,-
1.6662044083,-2.7411719796,2.2198726406\C,-1.1833672377,-
4.0030131277,2.570
3689535\C,-0.0471088537,-
4.4977946919,1.9344135691\C,0.5956404907,-3.7
358997767,0.957920384\H,-1.4119407471,-1.008423605,0.9876738869\H,-2.5
561376707,-2.3413031489,2.7005049502\H,-1.6867404888,-4.5916253384,3.3
327932633\H,0.345064557,-5.4761345723,2.1996749964\H,1.4833410953,-4.1
289349907,0.466246431\O,5.6770807063,-0.921520586,-0.2596936181\O,5.41
72143093,1.0619100609,-1.319379193\Version=EM64L-G09RevB.01\State=1-A
\HF=-1484.0300961\RMSD=2.546e-09\RMSF=2.380e-05\ZeroPoint=0.6315398\Th
ermal=0.6651418\Di pole=-8.8977098,0.0430335,1.0296017\PG=C01
[X(C31H38N1O3)]\\@
```

#### 14 (core)

```

1\1\GINC-V1296\FOpt\UM062X\Gen\C5H8N1O3(2)\GXG501\10-Feb-2013\0\#\M062
X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=6710886
40\ep_rcore+.freq\0,2\O,-0.0788507016,-0.033325346,1.0072034767\N,-1
.3084780191,-0.0823635885,0.7179600808\C,-1.9820716273,-1.3244952636,0
.3393994763\C,-2.2106165718,1.0632115527,0.8582697635\C,-3.4659258761,
-0.9536641175,0.4988299559\C,-3.5040504603,0.5564046943,0.2221818126\H
,-1.7730300832,1.9292609332,0.3554931148\H,-2.3277991155,1.3006125896,
1.924071055\H,-1.729873251,-1.5834849925,-0.6979827895\H,-1.6537854018
,-2.1359782275,0.9925177697\H,-4.3989559899,1.0309339891,0.6295693713\H
,-3.7684570595,-1.1618132611,1.5328796214\H,-3.4974572041,0.724167350
5,-0.859312438\C,-4.3652231977,-1.7543381524,-0.4084701302\O,-5.082539
6967,-1.3065999399,-1.2674269739\O,-4.2678602919,-3.0743667039,-0.1517
500837\H,-4.8607064523,-3.5401375166,-0.7680810827\Version=EM64L-G09R
evB.01\State=2-A\HF=-475.5275559\S2=0.755171\S2-1=0.\S2A=0.750018\RMSD
=3.457e-09\RMSF=5.506e-06\Di pole=-1.1245908,-0.327584,0.1246199\Quadru
pole=-9.0290685,7.6640396,1.3650289,0.2368756,-5.0409927,1.957524\PG=C
01 [X(C5H8N1O3)]\\@
```

#### 14

```

1\1\GINC-V1273\FOpt\UM062X\Gen\C13H24N1O3(2)\GXG501\11-Feb-2013\0\#\M0
62X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=67108
8640\ep_r+.freq\0,2\O,-0.0807750356,0.0874640342,1.0963449778\N,-1.2
941183759,-0.0449945504,0.7534200434\C,-1.8589755523,-1.346544835,0.30
3715001\C,-2.2320339051,1.092666551,0.8380924034\C,-3.3828793816,-1.05
74023358,0.4803061921\C,-3.5283798807,0.4682862893,0.3108011218\C,-1.7
205151998,2.2685927758,-0.0150526766\C,-2.3241136985,1.5703213164,2.30
01422536\C,-1.4917499895,-1.5990247773,-1.1728019171\C,-1.3169113886,-
2.4400964045,1.2352030368\C,0.0071767319,-1.7323214506,-1.4357733804\H
,-0.2287432527,-2.3265956653,1.2686404448\H,-1.91115901,-0.7900460827,
-1.7809251459\H,-1.6759310252,-2.2281209462,2.2497420222\H,-2.00421030
34,-2.5124193053,-1.5015700862\C,-1.6878471046,-3.8705997885,0.8485624
157\H,-0.8520454381,2.6941401604,0.5009473608\H,-1.3157846269,1.878483
9063,2.5990878735\H,-2.5034941975,3.0383070753,-0.0109260671\H,-2.9535
178561,2.4696883185,2.3121282922\C,-1.3241734713,1.9308051467,-1.44906
90903\C,-2.8563701351,0.5521552054,3.3039319108\H,-2.8405023159,0.9737
045692,4.3133446531\H,-3.8902435542,0.2597234468,3.0890446801\H,-2.234
9821807,-0.3491805938,3.3143661608\H,-0.9705543649,2.8313773583,-1.960
0867602\H,-0.5114163423,1.1981048632,-1.4646823692\H,-2.1604720341,1.5
319405074,-2.0328889576\H,0.1903300877,-1.8207035481,-2.5109948548\H,0
.5594307683,-0.8675406089,-1.0584594863\H,0.423267015,-2.6227116418,-0
.952766808\H,-1.2936649395,-4.5676056357,1.5942822425\H,-2.7708312491,
-4.0121309311,0.7963181728\H,-1.2603861569,-4.1525381421,-0.1193180175
\H,-4.4068312959,0.8474645262,0.8428113241\H,-3.6713946478,-1.37121276
09,1.4881094386\H,-3.6658230405,0.6894526701,-0.7513298085\C,-4.279224
8921,-1.7807957877,-0.5017636109\O,-4.5687807937,-1.3901159295,-1.6066
256602\O,-4.756667851,-2.942243986,-0.0086915901\H,-5.3155701156,-3.34
05740136,-0.6997837352\Version=EM64L-G09RevB.01\State=2-A\HF=-789.896
5042\S2=0.755177\S2-1=0.\S2A=0.750018\RMSD=3.572e-09\RMSF=1.140e-05\Di
pole=-0.9159578,-0.2839742,0.1879361\Quadrupole=-3.7597631,5.8599843,-
2.1002212,0.285431,-4.0525148,1.5748775\PG=C01 [X(C13H24N1O3)]\\@
```

#### 14-P (core)

```

1\1\GINC-X118\FOpt\RM062X\Gen\C9H15N1O3\GXG501\25-Jan-2013\0\#\M062X/g
en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=536870912\
\dep_core.freq\0,1\N,0.9832663324,0.4436095144,0.7607598929\C,2.00647
```

67516, 0.2634960983, 1.7896543866\c, 2.8675771595, 1.5110962652, 1.59552395  
 97\c, 1.8416250485, 2.5961726991, 1.1385996744\c, 0.5320888128, 1.829210416  
 4, 0.9362163262\o, -0.1130757705, -0.4113603813, 1.021864349\c, -0.47348251  
 4, -1.1169739935, -0.1618218234\h, -0.402366964, -0.4198929049, -1.00714903  
 06\c, -1.9206587454, -1.5576448991, 0.0285427439\c, 0.423394855, -2.3037821  
 128, -0.4197980793\h, -2.5728085996, -0.6877251176, 0.1460101337\h, -1.9981  
 808735, -2.1864372652, 0.9207376679\h, -2.2574336468, -2.1410373996, -0.833  
 7256309\h, -0.1035798362, 1.8994961208, 1.8317260978\h, -0.0286299802, 2.16  
 63971458, 0.0620794165\h, 1.5425852669, 0.2419150425, 2.790136116\h, 2.5509  
 271228, -0.6683793657, 1.6255226057\h, 3.6105594756, 1.3387716393, 0.812660  
 3896\h, 3.400266581, 1.8032654983, 2.5021022031\c, 2.3006705208, 3.31305293  
 2, -0.1102109189\o, 1.6898303654, 3.4215234803, -1.1440779727\o, 3.52222737  
 7, 3.8629296673, 0.0655400507\h, 3.7578499658, 4.3152491782, -0.7633705893\h,  
 0.4152370042, -2.6831765881, -1.441689332\c, 1.1483631253, -2.9167745582  
 , 0.5131316792\h, 1.154752907, -2.5594976234, 1.5395102074\h, 1.7477976789,  
 -3.7917772622, 0.2814353528\h, 1.7319467643, 3.365292129, 1.910363054\Version=EM64L-G09RevB.01\State=1-A\HF=-632.0878014\RMSD=6.794e-09\RMSF=3.  
 686e-06\Di pole=0.4421512, 0.1372175, 0.3749125\Quadrupole=1.0478212, 0.69  
 42705, -1.7420917, 2.2528245, 0.5648283, 3.0803135\PG=C01 [X(C9H15N1O3)]\\@

14-P

1\1\GINC-V1467\Freq\RM062X\Gen\C29H41N1O3\GXG501\12-Feb-2013\0\#M062X  
 /gen 6D SCF=Tight INT(grid=ultrafine) Freq=Noraman IOP(2/17=4) maxdisk  
 =3355443200\dep.freq\0,1\c,1.1103854838,0.552564874,0.6564204885\c,2  
 .0841075416,0.4988676302,1.8303837917\c,1.3470004969,1.7206854293,-0.2  
 740503723\h,1.7675334676,-0.3206506279,2.4893301306\c,3.5424697339,0.2  
 871264296,1.3934802026\h,2.0007808053,1.4237051094,2.4163762012\h,1.219  
 9792923,-0.3719467108,0.0794858079\c,1.6429614252,1.5012692651,-1.6198  
 338856\c,1.8459321999,2.5751852484,-2.4875475668\c,1.75139485,3.881165  
 468,-2.0112702016\c,1.459567966,4.1088680301,-0.6650573065\c,1.2632397  
 639,3.0337613905,0.1974230847\h,1.7017789886,0.4793827125,-1.990968972  
 7\h,2.0668735889,2.3912130469,-3.5351968056\h,1.9009509641,4.719739272  
 9,-2.6852615444\h,1.3813960607,5.1257728303,-0.2904302943\h,1.02135743  
 55,3.2120018275,1.2431523118\h,3.8451647666,1.1578847638,0.7961970324\c,  
 3.6816443236,-0.9401472409,0.5105248866\c,4.4606651274,0.2044769794,  
 2.6182525936\c,4.1808444847,-0.8327876092,-0.7896043275\c,4.2742657642  
 ,-1.9516046466,-1.6187543973\c,3.8644866118,-3.19990272,-1.1565002421\c,  
 3.3688083151,-3.3223856034,0.1422855859\c,3.2823602293,-2.2030261161  
 ,0.9663065775\h,4.485920832,0.1434881768,-1.1610254858\h,4.6631973413,  
 -1.8446520925,-2.6276124817\h,3.929571634,-4.0716018555,-1.8009515159\h,  
 3.0464506524,-4.2915936245,0.512678318\h,2.8888135152,-2.3137877756,  
 1.9750887868\h,4.3780707987,1.1124971194,3.2253504516\h,5.5054260515,0  
 .0837400633,2.3161940195\h,4.1924115056,-0.6496620788,3.2504371496\o,-  
 0.1885884797,0.5776483935,1.244105896\n,-1.1987092289,0.3605594286,0.2  
 736808618\c,-1.5439164721,-1.1044801088,0.1195938217\c,-2.3941284012,1  
 .1585347749,0.647778316\c,-3.1066440624,-1.065699313,0.0700977181\c,-3  
 .4725577174,0.4083141451,-0.1343064132\c,-2.2236838663,2.6190617009,0.  
 1988792329\c,-2.6776271957,1.1159993808,2.170965871\c,-0.9153216501,-1  
 .616869083,-1.1955409957\c,-1.0267549503,-1.9399503512,1.3075845232\c,  
 -1.2987903142,-0.828310038,-2.4463773531\h,0.0703934071,-1.918307658,1  
 .2897357281\h,-1.1844206949,-2.6681227347,-1.3307196065\h,-1.321272977  
 3,-1.4449678534,2.2395644943\h,0.1751051806,-1.5931859335,-1.078765385  
 8\c,-1.4898978059,-3.3972638926,1.3330999666\h,-1.4512177202,3.0728481  
 694,0.8348524445\h,-2.8638176434,0.079378069,2.4744491885\h,-3.1573733  
 671,3.1503161108,0.4203560936\h,-1.7671879675,1.4249084878,2.693378234  
 7\c,-1.863322782,2.8454889303,-1.267572032\c,-3.8479295078,1.983152587  
 3,2.643862783\h,-4.0761653275,1.7642833772,3.6917515305\h,-3.617086779  
 ,3.0500290134,2.5770828126\h,-4.7610766287,1.802061859,2.0658088671\h,  
 -1.7077081932,3.9139329741,-1.4503621711\h,-0.9426288873,2.3230308914,  
 -1.5351635804\h,-2.6581039379,2.5113147059,-1.9432721619\h,-0.77071498  
 71,-1.2254308049,-3.3193782948\h,-2.3715897919,-0.8921849237,-2.666199  
 0152\h,-1.0408630203,0.2285674091,-2.3357869998\h,-1.0612122619,-3.900  
 5871061,2.2058957131\h,-2.5786645731,-3.4853343032,1.3987730135\h,-  
 1.1790816139,-3.946343708,0.4405762074\h,-  
 4.4828837677,0.6388192644,0.212 9898339\h,-3.4759491381,-  
 1.3884441819,1.0540781618\h,-3.4214030413,0.6 613117965,-  
 1.1963392004\c,-3.78057829,-2.0239095793,-0.8869812775\o,-3  
 .4860649752,-3.1829794054,-1.0583087416\o,-4.8368691449,-1.4648583394,  
 -1.5182120176\h,-5.2364016895,-2.1621681171,-2.0677210879\Version=EM6  
 4L-G09RevB.01\State=1-A\HF=-1409.6016971\RMSD=3.981e-09\RMSF=1.558e-06

```
\ZeroPoint=0.6577569\Thermal=0.6908302\Di pole=0.004385,0.4526234,0.000
622\ PG=C01 [X(C29H41N1O3)]\
```

**14<sup>-</sup>** (core)

```
1\1\GINC-X10\FOpt\UM062X\Gen\C5H7N1O3(1-,2)\GXG501\27-Feb-2013\0\\#M06
2X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdisk
=536870912\\epc_rcore+.freq\\-1,2\N,-0.0204531234,0.1056427239,0.91237
12083\O,-1.2272362536,-0.0524998173,0.5501833717\C,0.8849166363,-1.023
8647845,1.1275377011\C,0.5388790612,1.3828375531,1.3832479132\C,2.2077
436364,-0.3339747792,1.453253379\C,1.7858993326,0.972213633,2.15898779
76\H,0.5079043565,-1.6256747559,1.9684948597\H,0.8943484424,-1.6515413
283,0.22992358\H,-0.2223922171,1.8952635571,1.9792535373\H,0.823059718
,2.0149181886,0.5332446411\H,2.871827025,-0.9369963458,2.0769406408\H,
2.7370241586,-0.0789044544,0.5266787244\H,1.5316656368,0.742301685,3.2
010141348\C,2.9613274018,2.0023797272,2.1457327264\O,2.9724040454,2.80
33995989,1.1830867748\O,3.7806221432,1.8609245984,3.0805750097\\Version
n=EM64L-G09RevB.01\HF=-474.9895311\S2=0.755416\S2-1=0.\S2A=0.75002\RMS
D=3.964e-09\RMSF=5.856e-06\Di pole=-1.5903097,-2.2969012,-0.358935\Quad
rupole=-16.6604233,7.379693,9.2807304,-27.4401955,-24.5514075,-13.7398
778\PG=C01 [X(C5H7N1O3)]\\@
```

**14<sup>-</sup>**

```
1\1\GINC-X127\FOpt\UM062X\Gen\C13H23N1O3(1-,2)\GXG501\02-Mar-2013\0\\#
M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxd
isk=536870912\\epc_r+.freq\\-1,2\O,-0.0593738783,0.122854832,1.0668301
062\N,-1.282877722,-0.0386321276,0.757067967\C,-1.8605860319,-1.346625
1984,0.3241810333\C,-2.233383168,1.0869603819,0.8483175541\C,-3.382015
3861,-1.0821289685,0.4957585957\C,-3.5356144571,0.4421227417,0.3613036
711\C,-1.7493595086,2.2600259123,-0.0259470008\C,-2.2897610622,1.58472
69708,2.3062538707\C,-1.4974516924,-1.6122121569,-1.1512380812\C,-1.30
19702193,-2.432196091,1.2568296686\C,-0.0010539974,-1.7484988189,-1.43
06545538\H,-0.2113164911,-2.3247058828,1.2905682069\H,-1.9328185415,-0
.815288065,-1.7619252373\H,-1.6650461063,-2.2163608948,2.2701050581\H,
-2.025796251,-2.5226265403,-1.457435574\C,-1.6960983175,-3.858492238
6,0.8725949205\H,-0.8733287883,2.7063824628,0.462350555\H,-1.279586740
9,1.9175359288,2.5761293648\H,-2.5450714798,3.0179451141,-0.0185163317
\H,-2.9403403625,2.470372758,2.325115429\C,-1.3838863073,1.9029499214,
-1.4639383575\C,-2.7737323891,0.5658166987,3.3336177803\H,-2.752516231
,0.9993574271,4.33993101\H,-3.797553807,0.2355845329,3.130870912\H,-2.
1278871011,-0.3178876984,3.3347096989\H,-1.0646966304,2.7999622967,-2.
0066882855\H,-0.5573740344,1.185447746,-1.4816736427\H,-2.2275780703,1
.4648157171,-2.0064430607\H,0.171648853,-1.8620192198,-2.507247622\H,0
.5568199098,-0.8751019596,-1.0786597079\H,0.4239187936,-2.6276966392,-
0.9321098291\H,-1.3701050884,-4.5584334118,1.6514155225\H,-2.779858796
5,-3.9414283415,0.736971131\H,-1.2174515652,-4.1643626274,-0.065086746
5\H,-4.400403856,0.8113699498,0.9254004166\H,-3.6630348785,-1.41480303
18,1.5014903899\H,-3.7240998578,0.6559571934,-0.6949696747\C,-4.288695
9151,-1.8675401659,-0.5197220511\O,-4.56538912,-1.270797443,-1.5845204
861\O,-4.6175383316,-3.0196980649,-0.152803619\\Version=EM64L-G09RevB.
01\HF=-789.358791\S2=0.755316\S2-1=0.\S2A=0.750019\RMSD=4.978e-09\RMSF
=2.413e-06\Di pole=2.2656331,2.2774869,1.5293266\Quadrapole=-32.6494607
,9.9569893,22.6924715,-31.5782841,-14.6741696,-4.040392\PG=C01 [X(C13H
23N1O3)]\\@
```

**14<sup>-P</sup>** (core)

```
1\1\GINC-X156\FOpt\RM062X\Gen\C9H14N1O3(1-)\GXG501\01-Mar-2013\0\\#M06
2X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdisk
=536870912\\dep c_core.freq\\-1,1\N,1.028096289,0.5731768621,0.66976304
54\O,2.1308601189,0.5509224469,1.5768127917\C,1.2213587114,1.663415054
9,-0.2825068266\C,-0.1885760611,0.949197716,1.4104506745\C,2.470126777
5,-0.7896612665,1.8721467845\H,1.5452929812,-1.3820195838,1.906817898\
C,3.1255025321,-0.7830117478,3.2513927361\C,3.3962878875,-1.3950217172
,0.844982025\H,4.0051477223,-0.1311710427,3.2367175346\H,2.4197583803,
-0.4105528847,3.9993833153\H,3.4456339571,-1.7918590894,3.5332085683\H
,3.5456703315,-2.4727829661,0.9291402393\C,4.0343414426,-0.7052819027,
-0.097426976\H,3.8842358169,0.3659907835,-0.1937030676\H,4.7045606699,
-1.1910643103,-0.800964708\C,-0.1868632041,1.8394532781,-0.855655089\C
,-1.1314790782,1.4560390341,0.3127989246\H,1.9766927706,1.3899686517,-
1.0265818935\H,1.5594253396,2.5704991483,0.2520797471\H,-0.617824911,0
.0910554568,1.9328442272\H,0.0754408946,1.7387067959,2.1353912182\H,-0
.3718612624,1.1553327173,-1.6875609077\H,-0.3488021606,2.857216643,-1.
2235003537\H,-1.6700027581,2.3384000039,0.6792125696\C,-2.2547296487,0
.4363369996,-0.0924362074\O,-2.6580532545,0.5327645609,-1.2737052111\O
```

```

,-2.6549232842,-0.3161306416,0.8255299412\Version=EM64L-G09RevB.01\HF
=-631.5387972\RMSD=3.328e-09\RMSF=4.548e-06\Dipole=5.0298691,0.3924015
,1.5105345\Quadrupole=-19.0704964,12.686647,6.3838493,-2.8655219,-5.76
99171,-0.0469992\PG=C01 [X(C9H14N1O3)]\@\@
```

**14^-P**

```

1\1\GINC-V1476\Freq\RM062X\Gen\C29H40N1O3(1-\GXG501\18-Mar-2013\0\#\#M
062X/gen 6D SCF=Tight INT(grid=ultrafine) Freq=Noraman IOP(2/17=4) Nos
ymm maxdisk=2013265920\depc.freq\,-1,\C,1.1019445025,0.5136127688,0.
7524633589\C,2.0778270739,0.5949593965,1.9262545402\C,1.3366146386,1.5
958423592,-0.2838334101\H,1.8411358385,-0.2220396034,2.6204647818\C,3.
5569880473,0.5225423778,1.5150647425\H,1.9001846469,1.5276211378,2.477
7499586\H,1.2346011739,-0.4530283446,0.2492716803\C,1.502794056,1.2461
224869,-1.6247171322\C,1.7376506719,2.2208118512,-2.5944410007\C,1.810
2616728,3.5634803199,-2.2284235701\C,1.646685656,3.9239389382,-0.89003
88599\C,1.4147547474,2.9448667644,0.0730944188\H,1.4289065882,0.198333
0095,-1.9093572465\H,1.8476914689,1.9311428187,-3.636006311\H,1.982775
3919,4.3273380462,-2.9819036174\H,1.6920577272,4.9701968284,-0.5986136
564\H,1.27760343707,3.2329601235,1.1130327081\H,3.7790004333,1.40528375
91,0.9007846906\C,3.8440647723,-0.7014244675,0.6648803184\C,4.45807451
09,0.5670335726,2.7548231545\C,4.3060348599,-0.5676063668,-0.646917637
2\C,4.5339947759,-1.6881288903,-1.4462341537\C,4.2992934488,-2.9652814
186,-0.9421820294\C,3.8412370971,-3.1130253525,0.3673709835\C,3.621157
8016,-1.9910856263,1.1619281146\H,4.4628500487,0.4294135496,-1.0537770
318\H,4.8814131845,-1.5600942831,-2.4679394493\H,4.4599357074,-3.83932
44225,-1.5668660125\H,3.6392884959,-4.1033808901,0.7660732724\H,3.2456
455997,-2.1221399261,2.1748693923\H,4.2694161701,1.4769650679,3.335622
7617\H,5.5158371313,0.5478628719,2.4725803713\H,4.2679098646,-0.292842
6193,3.4074463654\O,-0.1922599302,0.5539609672,1.33952829\N,-1.2029074
162,0.4001098842,0.345754752\C,-1.7028234277,-1.0260838831,0.20636969\
C,-2.3347114196,1.3067238021,0.66630827278\C,-3.2501066095,-0.838645963
6,0.1347678889\C,-3.4354529521,0.6423612951,-0.1650056334\C,-2.0086162
063,2.7492589666,0.2484346308\C,-2.6580596161,1.3152496104,2.186114838
5\C,-1.1036596549,-1.6123475917,-1.0893796962\C,-1.4009883707,-1.97831
55629,1.3868505748\C,-1.4577639359,-0.8688767969,-2.3775824898\H,-1.65
23813024,-1.4736459883,2.3263804251\H,-1.4446399955,-2.651609576,-1.16
42904366\H,-2.1262071129,-2.7902851155,1.2497984707\H,-0.0092186072,-1
.633501956,-0.9839676057\C,-0.0074839296,-2.5956286673,1.5195627806\H,
-1.1139854901,3.0567391392,0.8056590515\H,-2.4904336245,0.3189277382,2
.6026581239\H,-2.8243535419,3.3954683594,0.6023539261\H,-1.9308288496,
1.9720291256,2.6803009718\C,-1.7832986599,2.9902676946,-1.2412321324\C
,-4.0776384511,1.7606090426,2.5437887033\H,-4.1723046286,1.9029371915,
3.6265362476\H,-4.3475141645,2.7066004511,2.0601942724\H,-4.8173062733
,1.0121055316,2.2425404991\H,-1.4170509208,4.0093858472,-1.4123503795\
H,-1.0363528443,2.2946578577,-1.63414375\H,-2.7050023521,2.862425375,-
1.8176834693\H,-0.9355488959,-1.3254027751,-3.227981102\H,-2.531884674
7,-0.9122896116,-2.5820521548\H,-1.1548996747,0.1823286651,-2.31798402
28\H,-0.0064067938,-3.3146648534,2.3483996761\H,0.2900641442,-
3.141018216,0.618053366\H,0.7627154861,-1.851410796,1.7341042424\H,-
4.43818820
61,1.0057211517,0.0738566255\H,-3.6373157999,-
1.0381354021,1.146152423
3\H,-3.2789269573,0.8203315896,-
1.2319454946\C,-4.0202430925,-1.836193
2989,-0.7863757396\O,-
4.7916225759,-1.3282872152,-1.6303950557\O,-3.79
01688474,-
3.0480638538,-0.5505745314\Version=EM64L-G09RevB.01\HF=-140
9.0559372\RMSD=1.720e-09\RMSF=2.271e-06\ZeroPoint=0.6440511\Thermal=0.
6767066\Di
p
ole=6.6425404,3.2550011,1.7764559\PG=C01
[X(C29H40N1O3)]\@\@
```

**15 (core)**

```

1\1\GINC-X107\FOpt\UM062X\Gen\C9H8N1O3(2)\GXG501\10-Jan-2013\0\#\#M062X
/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=53687091
2\\tm_rcore+.freq\0,2\O,0.4661269015,0.0437073754,1.1243533964\N,-0.7
086257773,-0.2073155235,0.7339264372\C,-1.6996620022,0.8447585079,0.48
28280675\C,-1.2507426172,-1.5693554673,0.6910448469\C,-2.9323840865,0.
0426510357,0.1654419565\C,-2.6775980662,-1.3274989049,0.2837512507\C,-
4.1908751097,0.4991331497,-0.2003604683\C,-3.6780938791,-2.2625718313,
0.0378625694\H,-4.4027144764,1.5594550006,-0.2970049145\H,-3.479673642
6,-3.3267653396,0.1287440857\C,-5.196388054,-0.4411517022,-0.446351465
\C,-4.942572985,-1.8115810193,-0.3283763118\C,-6.5690728826,-0.0241272
538,-0.8428040257\H,-5.7504954884,-2.5081249613,-0.5291607885\O,-6.707
7327807,1.3149675427,-0.9279781917\O,-7.4812510508,-0.7831640462,-1.07
02198257\H,-1.8055129706,1.4696402309,1.3785718734\H,-1.3619591903,1.4
```

795282159, -0.3445571975\H, -0.6843595421, -2.1708633029, -0.0296481696\H,  
 -1.1553184964, -2.0347295995, 1.6804455988\H, -7.6280727508, 1.48944762, -1  
 .190333218\\Version=EM64L-G09RevB.01\\State=2-A\\HF=-627.9085847\\S2=0.75  
 5162\\S2-1=0.\\S2A=0.750018\\RMSD=8.153e-09\\RMSF=4.995e-06\\Dipole=-0.6886  
 471, 0.0560768, -0.1798155\\Quadrupole=-12.7378747, 10.6787804, 2.0590942, -  
 8.2128404, -4.0569629, -2.549633\\PG=C01 [X(C9H8N1O3)]\\@

**15**

1\\1\\GINC-X149\\FOpt\\UM062X\\Gen\\C13H16N1O3(2)\\GXG501\\10-Jan-2013\\0\\#M06  
 2X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=536870  
 912\\tm\_r+.freq\\0,2\\0,0.4288855443,0.0632589134,1.1798484287\\N,-0.767  
 0311757,-0.1921648894,0.8571404543\\C,-1.7372436476,0.8774844626,0.5268  
 104109\\C,-1.2811131522,-1.5796311993,0.7882272102\\C,-2.9612295716,0.04  
 60233254,0.2282748017\\C,-2.7080244448,-1.3195084192,0.3734016673\\C,-4.  
 2190411844,0.4963384255,-0.1493710543\\C,-3.7099801855,-2.2582200281,0.  
 1429006336\\H,-4.4298534139,1.5556248109,-0.2659926158\\H,-3.5133509052,  
 -3.3214747743,0.2557542397\\C,-5.2257864896,-0.4462695322,-0.3810059619  
 \\C,-4.9733622829,-1.8148574857,-0.2359327447\\C,-6.5964126777,-0.035580  
 4,-0.7881861118\\H,-5.7814769624,-2.514564729,-0.4249517022\\C,-1.170107  
 5121,-2.2352407071,2.1673226342\\C,-0.4888141257,-2.3670490639,-0.25887  
 98523\\C,-1.236865337,1.6641865734,-0.6872842405\\C,-1.9176627552,1.7958  
 204896,1.7381278676\\H,-0.1210348279,-2.2507995084,2.4769367652\\H,0.567  
 6360832,-2.3839544924,0.0244795356\\H,-0.2691358889,2.1172744382,-0.453  
 0037485\\H,-0.9564604369,2.2498777873,1.9961808845\\H,-1.544921442,-3.26  
 31734457,2.1293325846\\H,-0.8576161968,-3.3961630202,-0.317926859\\H,-1.  
 9477672427,2.4565744179,-0.94314837\\H,-2.635170118,2.5897755007,1.5067  
 351066\\H,-1.7500760449,-1.6775250568,2.9086435817\\H,-0.5837278778,-1.9  
 032281008,-1.2452015354\\H,-1.1195659892,1.0058457625,-1.5532172707\\H,-  
 2.2857301911,1.2314000955,2.6000828278\\O,-6.7347179336,1.3023382805,-0  
 .8992270656\\O,-7.5101558151,-0.7967778362,-1.0036465742\\H,-7.654718323  
 ,1.4701610623,-1.1667288394\\Version=EM64L-G09RevB.01\\State=2-A\\HF=-78  
 5.1075819\\S2=0.755256\\S2-1=0.\\S2A=0.750018\\RMSD=3.457e-09\\RMSF=6.255e-  
 06\\Dipole=-0.3740933,0.1056315,-0.1107491\\Quadrupole=-10.9232008,9.733  
 3506,1.1898502,-8.1726003,-3.1787122,-2.718104\\PG=C01 [X(C13H16N1O3)]\\@

**15-P (core)**

1\\1\\GINC-X153\\FOpt\\RM062X\\Gen\\C13H15N1O3\\GXG501\\09-Jan-2013\\0\\#M062X/  
 gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=536870912  
 \\dtm\_core.freq\\0,1\\C,1.6875376178,0.0968636623,0.6745985924\\C,2.7877  
 638348,-0.2433558562,1.6736748845\\C,1.8711806712,1.4893155398,0.121426  
 7917\\H,2.6861677562,-1.2761058868,2.01854594\\H,2.7226089767,0.42935518  
 26,2.534156773\\H,1.6963878281,-0.6246922657,-0.1530867963\\C,1.24032654  
 08,2.5700327823,0.5749573408\\H,0.5089238523,2.4965548701,1.3756205294\\  
 O,0.4559877281,-0.0527145349,1.3753745734\\N,-0.608444809,-0.2252522277  
 ,0.4620726721\\C,-1.6579643039,0.7785579657,0.7201234282\\C,-1.215465544  
 6,-1.5482053379,0.7038441863\\C,-2.8997024996,0.0470879453,0.2852709383  
 \\C,-2.6374216845,-1.3253864303,0.2695590311\\C,-4.1505298996,0.53487235  
 77,-0.0583669219\\C,-3.6214299319,-2.2390499671,-0.0884021037\\H,-4.3671  
 642477,1.5986230746,-0.0582032152\\H,-3.4159588838,-3.3057139219,-0.106  
 5153856\\C,-5.145152587,-0.3845155332,-0.4163913987\\C,-4.8833944219,-1.  
 758105674,-0.4314789\\C,-6.5103539507,0.0614578397,-0.8013401179\\H,-5.6  
 816159358,-2.4342486658,-0.7214376845\\O,-6.6595240938,1.4026850489,-0.  
 757747092\\O,-7.4144506207,-0.6737265076,-1.1238161589\\H,-7.5754992089,  
 1.5927587025,-1.0237485369\\H,3.7720521426,-0.1175015562,1.2127340902\\H  
 ,2.6122615731,1.5828327057,-0.6724350973\\H,1.4384104648,3.5556416793,0  
 .165274878\\H,-1.6966199887,1.0223459588,1.7949898153\\H,-1.4565250154,1  
 .6922672648,0.155221914\\H,-0.6870218295,-2.3222592767,0.1394095194\\H,-  
 1.1669095296,-1.7974389381,1.7766535109\\Version=EM64L-G09RevB.01\\Stat  
 e=1-A\\HF=-784.4683438\\RMSD=7.644e-09\\RMSF=1.404e-05\\Dipole=0.7745446,0  
 .2077425,0.144961\\Quadrupole=-2.0363385,5.9506378,-3.9142994,-7.513100  
 8,-3.0851317,-1.7254665\\PG=C01 [X(C13H15N1O3)]\\@

**15-P**

1\\1\\GINC-X148\\Freq\\RM062X\\Gen\\C29H33N1O3\\GXG501\\09-Feb-2013\\0\\#M062X/  
 gen 6D SCF=Tight INT(grid=ultrafine) IOP(2/17=4) Freq=Noramman maxdisk=536870912\\dtm.freq\\0,1\\C,1.675615485,0.2470362626,0.6746783817\\C,2.7  
 337792457,-0.1576250133,1.6975261398\\C,1.8622936019,1.6492176568,0.139  
 3775475\\H,2.4946938637,-1.1717823656,2.0452636494\\C,4.1676256196,-0.11  
 53363099,1.1478554853\\H,2.6618127322,0.4996594185,2.5738481029\\H,1.688  
 2570218,-0.4546264814,-0.1671314192\\C,2.0257732943,1.8728622208,-1.227  
 1546048\\C,2.1520971855,3.1711857781,-1.7237505269\\C,2.113426877,4.2573  
 242304,-0.852146148\\C,1.9532351515,4.0413487791,0.5185330144\\C,1.83121

19163, 2.7445081253, 1.0092833924\H, 2.0383003649, 1.0229197932, -1.9062847  
 952\H, 2.2695141134, 3.3336520197, -2.7914478452\H, 2.2041231987, 5.2690410  
 46, -1.2367603137\H, 1.9186550707, 4.8854222902, 1.2015900992\H, 1.68466597  
 48, 2.578240216, 2.0745462235\H, 4.3889868532, 0.9230437889, 0.8668420139\C  
 , 4.3141674326, -0.9647478435, -0.1016246131\C, 5.1663363047, -0.5394064687  
 , 2.2312862302\C, 4.728386995, -0.3957365427, -1.3083489293\C, 4.8499867686  
 , -1.1689467668, -2.463603903\C, 4.5556510119, -2.5297857972, -2.4275406188  
 \C, 4.1444772188, -3.1117876776, -1.227880004\C, 4.0275989309, -2.335343870  
 3, -0.0776826763\H, 4.9474655743, 0.6695351062, -1.3441583497\H, 5.17268786  
 42, -0.7053900805, -3.3917248855\H, 4.6460614555, -3.1340716732, -3.3253747  
 244\H, 3.9144870075, -4.1729278433, -1.1887925238\H, 3.7051565579, -2.80366  
 11876, 0.8505443224\H, 5.0839204315, 0.1109599711, 3.10882497\H, 6.19334982  
 81, -0.4881275232, 1.8572576279\H, 4.9778035864, -1.5691386924, 2.555717050  
 6\O, 0.4171893364, 0.1172157646, 1.3484784939\N, -0.6235811775, -0.12606619  
 14, 0.4326607331\C, -1.7104302449, 0.8960041729, 0.5229172367\C, -1.1611431  
 187, -1.5042434308, 0.6338852711\C, -2.9056608509, 0.0464022617, 0.14939748  
 64\C, -2.5887782446, -1.3097267261, 0.18743295\C, -4.1839795435, 0.46379980  
 6, -0.195842453\C, -3.5405992399, -2.2774104053, -0.121536296\H, -4.4472858  
 009, 1.5169849619, -0.2335971251\H, -3.2910482515, -3.3352885406, -0.094940  
 7156\C, -5.1447043261, -0.5064361841, -0.5022761969\C, -4.82505331, -1.8684  
 083467, -0.4675970062\C, -6.5326229322, -0.1326179872, -0.8800940405\H, -5.  
 5973253363, -2.5893903432, -0.7170118543\C, -1.126294828, -1.9938970792, 2.  
 0908481641\C, -0.3770367035, -2.475583209, -0.2500833549\C, -1.4710783257,  
 2.0066519075, -0.5034126518\C, -1.876176748, 1.5133771017, 1.918382002\H, -  
 0.0948478795, -2.067066053, 2.4452957389\H, 0.6676199315, -2.5242068431, 0.  
 080050544\H, -0.5989940539, 2.6083564313, -0.2310159354\H, -0.9788154181, 2  
 .0767904951, 2.1888584361\H, -1.5897005527, -2.9849042189, 2.1456730721\H,  
 -0.794261373, -3.4868290778, -0.184612271\H, -2.3405269114, 2.672789978, -0  
 .5476291919\H, -2.7301913193, 2.1992414102, 1.9078571244\H, -1.6757431603,  
 -1.3259643668, 2.75795298\H, -0.3991718169, -2.1464508607, -1.2925071215\H  
 , -1.3042785579, 1.5754935188, -1.4944497146\H, -2.0562506574, 0.7561117202  
 , 2.6848137943\O, -6.7394893264, 1.2021233906, -0.883753062\O, -  
 7.4102847273, -0.9160944028, -1.1604413887\H, -  
 7.6668938911, 1.3409411866, -1.14143184

32 \Version=EM64L-G09RevB.01\State=1-A\HF=-1404.8171601\RMSD=7.660e-09 \RMSF=2.558e-06\ZeroPoint=0.5644321\Thermal=0.5951411\Di pole=0.9852808

, 0.4423218, 0.159276\ PG=C01 [X(C29H 33N1O3)]\\@

**15<sup>-</sup>** (core)

1\1\GINC-X151\FOpt\UM062X\Gen\C9H7N1O3(1-,2)\GXG501\11-Jan-2013\0\\#M0  
 62X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=53687  
 0912\\tmc\_rcore+.freq\\-1,2\O, 0.4919904485, 0.03631786, 1.1156189834\N, -  
 0.7003382914, -0.2129163952, 0.7684617442\C, -1.6903954565, 0.8352839763, 0  
 .4944313868\C, -1.2324728435, -1.5771557261, 0.6847950162\C, -2.9261253931  
 , 0.0332710258, 0.1798692325\C, -2.6641488096, -1.3349446564, 0.2883043672\  
 C, -4.1905976981, 0.490104024, -0.1763582693\C, -3.6720389231, -2.262323708  
 9, 0.0394508105\H, -4.4305023784, 1.546519815, -0.2708753355\H, -3.47405742  
 49, -3.3297883816, 0.1216635742\C, -5.2096195427, -0.4311400164, -0.4277632  
 263\C, -4.9392741648, -1.7998842585, -0.3170799994\C, -6.6274334273, 0.0620  
 917811, -0.8265947635\H, -5.7590773528, -2.4827671787, -0.5214734681\O, -6.  
 7521629506, 1.3046902247, -0.8944749201\O, -7.4645695523, -0.8441932953, -1  
 .029273003\H, -1.7923008827, 1.4761369903, 1.3797355731\H, -1.3399064264, 1  
 .4561558111, -0.3395662734\H, -0.6535906463, -2.1460156474, -0.0545647119\  
 H, -1.1171033261, -2.0687067574, 1.6601876499\Version=EM64L-G09RevB.01\S  
 tate=2-A\HF=-627.3711663\S2=0.755268\S2-1=0.\S2A=0.750019\RMSD=7.544e-09\RMSF=2.381e-06\Di pole=4.0566711, -1.2947097, 1.138666\Quadrupole=-37.  
 7570471, 19.7645156, 17.9925315, 4.1328545, -16.4867826, 1.1907406\PG=C01 [X(C9H7N1O3)]\\@

**15<sup>-</sup>**

1\1\GINC-X119\FOpt\UM062X\Gen\C13H15N1O3(1-,2)\GXG501\10-Jan-2013\0\\#M0  
 62X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=536  
 870912\\tmc\_r+.freq\\-1,2\O, 0.439835954, 0.0606327034, 1.1878870622\N, -0  
 .7585076626, -0.1948095152, 0.8616934793\C, -1.7342417759, 0.869761882, 0.5  
 246153648\C, -1.2756869648, -1.5820371928, 0.7920961807\C, -2.9589802971, 0  
 .0389378452, 0.2231491804\C, -2.7024304485, -1.3239276415, 0.37230247\C, -4  
 .2185303753, 0.4891395889, -0.1598928386\C, -3.7110524764, -2.255352686, 0  
 .1378665574\H, -4.4555207163, 1.5437983286, -0.2862420065\H, -3.5180032857  
 , -3.3216264591, 0.2522631555\C, -5.2383284075, -0.4346212718, -0.397932978  
 1\C, -4.9732838695, -1.8007239972, -0.2461851203\C, -6.6493066207, 0.052566  
 2163, -0.8260667295\H, -5.7925258978, -2.4872528323, -0.4405209713\C, -1.15  
 95240564, -2.2347473366, 2.1723787769\C, -0.472318709, -2.3695333228, -0.24

67815602\c,-1.2303752359,1.6571514208,-0.6872477427\c,-1.9177520644,1.  
 7928736045,1.7317131604\h,-0.1101429915,-2.2616734888,2.4839763488\h,0  
 .5833404018,-2.3977861594,0.0427209124\h,-0.2719225848,2.1313834522,-0  
 .4516170434\h,-0.9645648332,2.2680068976,1.9861269638\h,-1.5494287495,  
 -3.2576383101,2.1353050398\h,-0.8535403392,-3.3941078935,-0.3147565458  
 \h,-1.9594505104,2.4283963943,-0.9557147368\h,-2.6561222626,2.56610518  
 65,1.4964019734\h,-1.7376388954,-1.670327089,2.9101770954\h,-0.5610303  
 116,-1.9010091494,-1.231539919\h,-1.0994557842,0.9923295587,-1.5464904  
 796\h,-2.2766220598,1.2247816526,2.5953704888\o,-6.7684365353,1.293483  
 747,-0.9296876665\o,-7.4881616699,-0.8554994202,-1.0132285593\version  
 =EM64L-G09RevB.01\State=2-A\HF=-784.5686443\S2=0.755342\S2-1=0.\\$2A=0.  
 750019\RMSD=6.861e-09\RMSF=8.193e-06\Di pole=5.2753002,-1.1518387,1.564  
 2586\Quadrupole=-43.9135598,23.5995624,20.3139974,5.2051173,-20.194335  
 1,1.6259556\PG=C01 [X(C13H15N1O3)]\\@

**15^-P (core)**

1\1\GINC-X126\FOpt\RM062X\Gen\C13H14N1O3(1-)\GXG501\10-Jan-2013\0\\#M0  
 62X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=53687  
 0912\dtmc\_core.freq\|-1,1\c,1.6916103678,0.0994580713,0.696553177\c,2  
 .7745976725,-0.2875003263,1.7002525166\c,1.943885516,1.4825411353,0.14  
 57238855\h,2.6255608982,-1.3159537035,2.0416941266\h,2.7292924429,0.38  
 37257085,2.563555492\h,1.6820593895,-0.6191972706,-0.134843442\c,1.291  
 3531373,2.5773661072,0.5288313258\h,0.4898803452,2.5204829761,1.259907  
 8156\o,0.4560372086,0.0010122854,1.3828731529\n,-0.6046791822,-0.17994  
 9185,0.4532833885\c,-1.6738764931,0.8051377852,0.7167998106\c,-1.19506  
 19961,-1.5164044439,0.6773200233\c,-2.909034489,0.0580712342,0.2831249  
 488\c,-2.6227674213,-1.3071942103,0.2499999625\c,-4.1740214162,0.53170  
 15678,-0.042996721\c,-3.6041961871,-2.2230999186,-0.1126721338\h,-4.43  
 0849098,1.5882770186,-0.0355472607\h,-3.385477445,-3.2892619318,-0.148  
 3377149\c,-5.1730822421,-0.3785466402,-0.4027020717\c,-4.8772283796,-1  
 .7457402005,-0.4349059862\c,-6.5944148548,0.1269543544,-0.7701207076\h  
 ,-5.6800244282,-2.4167684063,-0.7274256754\o,-6.7462428158,1.367437892  
 5,-0.7078895337\o,-7.4123596977,-0.7669557799,-1.0813139882\h,3.767643  
 5982,-0.2016533985,1.2471415644\h,2.7463408601,1.5537443892,-0.5898134  
 477\h,1.5312604514,3.5534332928,0.1177170548\h,-1.7025122456,1.0481740  
 127,1.7927369615\h,-1.4877337979,1.7231865194,0.1517940377\h,-0.651112  
 4468,-2.2714614696,0.0983320814\h,-1.1243572515,-1.7771874655,1.746727  
 3575\version=EM64L-G09RevB.01\State=1-A\HF=-783.9235246\RMSD=4.320e-0  
 9\RMSF=8.219e-06\Di pole=7.8849376,-0.638154,1.704234\Quadrupole=-50.54  
 41963,27.6344066,22.9097898,3.4416609,-20.9678086,0.6957488\PG=C01 [X  
 C13H14N1O3)]\\@

**15^-P**

1\1\GINC-X129\Freq\RM062X\6-31+G(d)\C29H32N1O3(1-)\GXG501\16-Jan-2013\0\\#M062X/6-31+G(d) 6D SCF=Tight INT(grid=ultrafine) IOP(2/17=4) Freq=Noraman maxdisk=2013265920\dtmc.geom.freq\|-1,1\c,1.6552602481,0.2456  
 168616,0.6661982719\c,2.7157259074,-0.1607876752,1.6884708344\c,1.8679  
 26486,1.641451738,0.1193769125\h,2.4769772217,-1.1770880218,2.03016379  
 3\c,4.1542041639,-0.1040426789,1.1549519078\h,2.6329141023,0.491256337  
 8,2.5681588384\h,1.6572087318,-0.4622319969,-0.1710351212\c,2.07510681  
 17,1.8513516452,-1.243193566\c,2.2341744945,3.1433596001,-1.7468121306  
 \c,2.1847542404,4.2378188285,-0.886376182\c,1.9769567323,4.0358464695,  
 0.4799730665\c,1.8214933713,2.7452648365,0.977346743\h,2.0887560631,0.  
 9958184557,-1.915110684\h,2.3782461875,3.2946137797,-2.8131306989\h,2.  
 2949776457,5.2453738256,-1.2775914566\h,1.9231321509,4.8868818765,1.15  
 34693456\h,1.6277376618,2.588444187,2.0364463604\h,4.3764801494,0.9407  
 53798,0.8993781324\c,4.3286219158,-0.9249678453,-0.1095715334\c,5.1431  
 151524,-0.5499997428,2.2394272464\c,4.8150859815,-0.3379629905,-1.2802  
 472388\c,4.9729554602,-1.0851530949,-2.4479180014\c,4.6415323843,-2.43  
 79224591,-2.4616689732\c,4.1552485296,-3.0371475083,-1.299257423\c,4.0  
 04183786,-2.2868990366,-0.135948404\h,5.054445825,0.723551308,-1.27973  
 24137\h,5.3460603827,-0.6058570038,-3.3489699893\h,4.7530106398,-3.020  
 631139,-3.3715264296\h,3.8847177097,-4.089416641,-1.3012324828\h,3.614  
 4067164,-2.7660313636,0.7601389926\h,5.0428490847,0.0751035278,3.13365  
 01389\h,6.1753730305,-0.4815316706,1.8812630239\h,4.9564864228,-1.5898  
 403687,2.5319172416\o,0.4065393587,0.1406247242,1.3446548058\n,-0.6381  
 195932,-0.1404514148,0.4329983505\c,-1.7318767597,0.8794309606,0.48375  
 77093\c,-1.1741811469,-1.5118975389,0.683736623\c,-2.9273197667,0.0142  
 54426,0.1426665856\c,-2.6037356327,-1.3362357896,0.2312233907\c,-4.211  
 9294222,0.4167181085,-0.2105574295\c,-3.5632696517,-2.3091787232,-0.03  
 73561413\h,-4.5047438631,1.4616935158,-0.2911333994\h,-3.3155336373,-3  
 .3683831353,0.0280469536\c,-5.1872702597,-0.5472949637,-0.4773344889\c

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,-4.8512320166,-1.9034932952,-0.3909683799\c,-6.6268094086,-0.11605846
13,-0.8667730102\h,-5.635933531,-2.6219155278,-0.6111661015\c,-1.12218
91384,-1.9502422069,2.1563068647\c,-0.3835206992,-2.5093158349,-0.1661
066618\c,-1.4898396128,1.952121173,-0.5812875391\c,-1.8961869177,1.550
5290303,1.8540931825\h,-0.0888443218,-2.027079673,2.5096785096\h,0.662
8163297,-2.5522021963,0.1656511654\h,-0.6247197947,2.5751531324,-0.328
9419992\h,-1.0098451605,2.1433487443,2.1034749835\h,-1.6020602954,-2.9
310594598,2.2467569179\h,-0.806925356,-3.5162080617,-0.0725359354\h,-2
.3691971398,2.600837116,-0.6604828989\h,-2.766706058,2.2139141121,1.81
65709516\h,-1.6612737352,-1.2529258386,2.8015070855\h,-0.4086007139,-2
.2114245346,-1.2179937767\h,-1.3162742902,1.4805953393,-1.5528352086\h
,-2.0638064279,0.8188024818,2.6481055307\o,-6.815740892,1.1202999855,-
0.9064723461\o,-7.4203288366,-1.0567070329,-1.0913174143\\Version=EM64
L-G09RevB.01\State=1-A\HF=-1404.2712819\RMSD=2.263e-09\RMSF=1.903e-06\
ZeroPoint=0.5504126\Thermal=0.5809718\Di pole=11.7534509,0.0265885,1.49
67662\PG=C01 [X(C2 9H32N1O3)]\\@
```

**13 (core)**

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1\1\GINC-X151\FOpt\UM062X\Gen\C10H16N1O5(2)\GXG501\10-Dec-2012\0\\#M06
2X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=536870
912\phehe_r+.freq\0,2\N,-0.0000003545,-0.0000000601,0.0031316915\o,-
0.0000005332,-0.000001266,1.2679713097\c,1.2573898867,0.0301137515,-0
.7761292769\c,-1.2573903755,-0.0301137897,-0.7761296353\c,0.7137971845
,-0.2719675948,-2.1937136765\c,-0.7137972727,0.2719677057,-2.193713849
5\c,1.5468520265,0.3317613367,-3.297212671\c,-1.5468518029,-0.33176110
97,-3.2972131429\h,0.6996475504,-1.3571657584,-2.3499242151\h,-0.69964
75945,1.3571658858,-2.34992427\c,1.879866498,1.4253292199,-0.653563632
6\c,-1.8798670214,-1.4253292711,-0.6535643137\c,2.2121472025,-1.039091
1605,-0.2580183932\c,-2.2121478376,1.0390910678,-0.258018909\h,1.23159
50117,2.1953499552,-1.0854693379\h,-1.231595413,-2.1953499609,-1.08546
99169\h,2.8491733092,1.4588615543,-1.1621074828\h,-2.8491736889,-1.458
861552,-1.1621084413\h,2.0313479796,1.6524821926,0.4054686402\h,-2.031
3488022,-1.6524823551,0.4054678924\h,1.7376200734,-2.0251685945,-0.287
9359106\h,-1.7376207001,2.0251685049,-0.2879361885\h,3.1147805798,-1.0
61611507,-0.8752407298\h,-3.1147810405,1.0616114791,-0.8752414982\h,2.
4860077103,-0.8190341509,0.7771516824\h,-2.486008638,0.8190339493,0.77
71510661\o,-2.7490683464,0.266803142,-3.3974124076\o,-1.2130499773,-1.
2502543944,-4.0041457036\h,-3.2327012175,-0.1667192289,-4.123172848\o,
2.7490685983,-0.2668029045,-3.3974116589\o,1.2130504006,1.2502546957,-
4.0041452293\h,3.2327016745,0.1667195427,-4.123171917\\Version=EM64L-G
09RevB.01\State=2-B\HF=-821.2399937\S2=0.755223\S2-1=0.\S2A=0.750018\R
MSD=5.431e-09\RMSF=2.501e-05\Di pole=0.,0.,-0.5277758\Quadrupole=11.913
9127,-2.354322,-9.5595907,1.1261904,0.0000031,0.0000005\PG=C02 [C2(N1O
1),X(C10H16O4)]\\@
```

**13**

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1\1\GINC-D19\FOpt\UM062X\Gen\C6H8N1O5(2)\ETS502\29-May-2013\0\\#M062X/
gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdisk=16
10612736\phehe_r_core.freq\0,2\N,-0.0000036769,-0.0000014356,-0.0063
477443\o,-0.0000071544,-0.0000054032,1.2569314399\c,1.2293562647,0.016
247869,-0.7995085241\c,-1.2293591558,-0.0162461155,-0.7995155217\c,0.7
114627074,-0.282122901,-2.214468229\c,-0.7114576962,0.2821328656,-2.21
44707177\c,1.5700697611,0.324811538,-3.2962824302\c,-1.5700579742,-0.3
247941098,-3.2962944775\h,0.6804524653,-1.3654742633,-2.3768622324\h,-
0.6804467713,1.3654850778,-2.3768584498\h,1.7021408813,1.00513876,-0.7
273131725\h,-1.7021441078,-1.005137451,-0.7273283979\h,1.9252419811,-0
.7343226435,-0.4187856416\h,-1.9252469984,0.7343221652,-0.4187920896\o
,-2.7928798598,0.2338822401,-3.3207236864\o,-1.2344619693,-1.213846002
8,-4.0380554719\h,-3.3028490322,-0.1969982223,-4.0297931432\o,2.792878
1031,-0.233893488,-3.3207355102\o,1.2344693286,1.2138496801,-4.0380579
092\h,3.3028429037,0.1969738404,-4.0298160908\\Version=EM64L-G09RevC.0
1\HF=-664.039878\S2=0.755146\S2-1=0.\S2A=0.750018\RMSD=2.855e-09\RMSF=
1.749e-05\Di pole=0.000002,0.0000039,-0.7884359\Quadrupole=10.256268,-2
.9842609,-7.2720071,0.9434509,0.0000172,0.0000367\PG=C01 [X(C6H8N1O5)]\\@
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**13- (core)**

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1\1\GINC-X113\FOpt\UM062X\Gen\C10H15N1O5(1-,2)\GXG501\11-Dec-2012\0\\#M062X/
gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=536
870912\phece_r+.freq\0,2\N,-0.0104050085,0.105091665,0.0303965855\o,-
0.0105935755,0.1057429003,1.2995973751\c,1.2545880295,0.061229709,-0
.7382176772\c,-1.2510113059,0.0188780642,-0.7817030192\c,0.7183689825,
-0.2652685966,-2.1536261738\c,-0.7037598044,0.295028869,-2.1912509674\@
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C,1.5757070013,0.2824195913,-3.2603613597\c,-1.5489372325,-0.290929610
3,-3.3666662861\h,0.6794894067,-1.350726981,-2.2860672417\h,-0.6526308
194,1.382664391,-2.3398541753\c,1.9366383929,1.4287896119,-0.625384725
6\c,-1.836007224,-1.3906537473,-0.6337741682\c,2.1608385816,-1.0345203
609,-0.1829049017\c,-2.2554640892,1.0624213036,-0.3127715601\h,1.33409
82569,2.2095730763,-1.0983757803\h,-1.1474641968,-2.1471491165,-1.0276
766185\h,2.9182530302,1.4127636512,-1.1128050824\h,-2.7685467496,-1.44
93785733,-1.2009147263\h,2.0690320463,1.6682345818,0.4347429582\h,-2.0
197891928,-1.5999007016,0.4257978778\h,1.6386373631,-1.9968513098,-0.1
825837937\h,-1.8030474638,2.0605438446,-0.3275735168\h,3.056906628,-1.
1233146209,-0.8067756971\h,-3.1033271131,1.0434808631,-1.0036123712\h,
2.4546836752,-0.7986245555,0.8444027464\h,-2.5884522474,0.8453756448,0
.7076836465\o,-0.8887255456,-0.9045739792,-4.2355507295\o,-2.777248586
5,-0.0630977445,-3.3000565807\o,2.5014917789,-0.6121032685,-3.68452293
73\o,1.5407709245,1.405831645,-3.7053972978\h,2.9750920574,-0.18209724
62,-4.4168048017\\Version=EM64L-G09RevB.01\\State=2-A\\HF=-820.7059144\\S
2=0.755378\\S2-1=0.\$2A=0.750019\\RMSD=2.513e-09\\RMSF=6.529e-06\\Dipole=2
.8220846,0.2635858,1.9927496\\Quadrupole=1.7327092,10.7906339,-12.52334
32,-2.3961916,-12.3188021,-2.9309143\\PG=C01 [X(C10H15N1O5)]\\@
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13<sup>-</sup>

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1\\1\\GINC-D18\\FOpt\\UM062X\\Gen\\C6H7N1O5(1-,2)\\ETS502\\29-May-2013\\0\\#M06
2X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdisk
=1610612736\\pcece_r_core.freq\\-1,2\\N,-0.0413859508,0.0733452663,0.05
25205345\o,-0.0628143387,0.1380037832,1.3190851984\c,1.2082902912,0.09
1909956,-0.7102781813\c,-1.2403548935,0.049064659,-0.7967422225\c,0.74
29688437,-0.3012219709,-2.115811303\c,-0.6788499441,0.2909950591,-2.19
26549468\c,1.6270365372,0.2454269393,-3.2035474028\c,-1.4846995045,-0.
3092778257,-3.3797772127\h,0.6913746072,-1.3897806763,-2.2152235429\h,
-0.5746085286,1.3706882647,-2.3665729365\h,1.6338508157,1.1053474599,-
0.7000831577\h,-1.735151559,-0.927483372,-0.7270407857\h,1.918980167,-
0.6018205398,-0.2502867673\h,-1.9410428459,0.8150488365,-0.4556698461\
o,-0.7982024009,-0.4662356743,-4.4170363945\o,-2.6913738949,-0.5441189
605,-3.1615236888\o,2.273308016,-0.7153572111,-3.8935318786\o,1.823304
5707,1.4222995978,-3.4102788914\h,2.735918012,-0.2636585912,-4.6193835
745\\Version=EM64L-G09RevC.01\\HF=-663.5094158\\S2-1=0.\$2A=
0.75002\\RMSD=2.513e-09\\RMSF=2.382e-05\\Dipole=2.7070944,0.2528857,1.087
665\\Quadrupole=9.1786646,19.1358211,-28.3144857,-5.9562644,-18.8831353
,-3.7678197\\PG=C01 [X(C6H7N1O5)]\\@
```

13<sup>2-</sup> (core)

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1\\1\\GINC-X105\\FOpt\\UM062X\\Gen\\C10H14N1O5(2-,2)\\GXG501\\11-Dec-2012\\0\\#
M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=536
870912\\pcece_r+.freq\\-2,2\\N,0.0071795678,-0.0124230343,-0.0141147303
\o,0.0071961589,-0.0242884744,1.2604562249\c,1.2522137463,0.0199650317
,-0.8092817107\c,-1.237849987,-0.0299311654,-0.8096549585\c,0.73507993
54,-0.230921905,-2.25006568\c,-0.7208089479,0.2476309423,-2.2455803615
\c,1.718657625,0.4516649269,-3.2542163616\c,-1.7044450251,-0.416190293
9,-3.2621842122\h,0.7519227791,-1.3085321662,-2.4518026162\h,-0.737638
2598,1.328798996,-2.4272956998\c,1.8886188922,1.4055092866,-0.62432145
48\c,-1.8741573851,-1.4186791404,-0.650319038\c,2.2124692175,-1.064099
488,-0.3293594185\c,-2.1980528232,1.0450269946,-0.3095860814\h,1.23975
65957,2.1830324439,-1.0398839101\h,-1.2253221341,-2.1883484349,-1.0803
009094\h,2.8429609709,1.4436788684,-1.1596419327\h,-2.8285611259,-1.44
69315538,-1.1861394312\h,2.048038876,1.5893789315,0.4456905044\h,-2.03
34395579,-1.6223614885,0.4161196365\h,1.7130945145,-2.0401120227,-0.33
93490834\h,-1.6986892586,2.0210631009,-0.3015117057\h,3.0559519051,-1.
0919533723,-1.0268811535\h,-3.04160081,1.085797692,-1.0063906235\h,2.5
588225125,-0.8570000209,0.6909458114\h,-2.544304095,0.819025317,0.7067
361947\o,-1.358667914,-1.499018184,-3.7847581581\o,-2.8097356499,0.182
7682073,-3.3758162776\o,2.8240709094,-0.1448890906,-3.3787751459\o,1.3
726493018,1.5438046401,-3.7568832888\\Version=EM64L-G09RevB.01\\State=2
-A\\HF=-820.05765\\S2=0.755494\\S2-1=0.\$2A=0.75002\\RMSD=7.688e-09\\RMSF=9
.454e-06\\Dipole=0.000355,-0.0394395,4.3301409\\Quadrupole=-8.8799853,20
.1786211,-11.2986358,-5.0403334,-0.0512106,0.2965708\\PG=C01 [X(C10H14N
1O5)]\\@
```

13<sup>2-</sup>

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1\\1\\GINC-D19\\FOpt\\UM062X\\Gen\\C6H6N1O5(2-,2)\\ETS502\\29-May-2013\\0\\#
M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdisk
=1610612736\\pcece_r_core.freq\\-2,2\\N,0.0072295033,-0.0126990474,-0.0
290691415\o,0.0072981085,-0.0242919165,1.2456455994\c,1.2258271294,-0.
0093081921,-0.8362792005\c,-1.2114667901,-0.0002451797,-0.8360621968\c
```

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, 0.7385838119, -0.2328725453, -2.2788798601\c, -0.7243204823, 0.2502071882
, -2.2743062227\c, 1.7491206501, 0.5101498023, -3.2106148048\c, -1.73487808
48, -0.4754310366, -3.2196293064\h, 0.7546327639, -1.3009126744, -2.5169970
4\h, -0.7404720417, 1.3224910337, -2.4924955148\h, 1.7165896559, 0.96921412
05, -0.7240855285\h, -1.7027759894, -0.9804136545, -0.7422312795\h, 1.90705
90835, -0.7828987517, -0.4662737792\h, -1.8922035916, 0.7666548738, -0.4514
746675\o, -1.4514310052, -1.6423375601, -3.5796621424\o, -2.7947733364, 0.1
687730955, -3.440175933\o, 2.8092748107, -0.1296491062, -3.4424914864\o, 1.
4654098043, 1.6832725503, -3.5495974952\Version=EM64L-G09RevC.01\HF=-66
2.8576888\S2=0.755518\S2-1=0.\S2A=0.750021\RMSD=9.902e-09\RMSF=7.709e-
06\Dipole=-0.0000052,-0.0277231,2.988638\Quadrupole=6.5684151,34.49203
57,-41.0604508,-6.9479134,0.080504,0.4485777\PG=C01 [X(C6H6N1O5)]\@\n

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**13-P (core)**

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1\1\GINC-D16\FOpt\RM062X\Gen\C26H33N1O5\ETS502\31-May-2013\0\#M062X/g
en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdisk=348
9660928\sty_phehe_opt.freq\0,1\N,1.2996460135,-0.1292584572,-0.06448
22211\o,0.0218261611,-0.2404206959,0.5191235961\c,1.8818582011,-1.4828
162071,-0.234756355\c,2.2117834864,0.759170798,0.7285916499\c,3.360896
837,-1.0789893707,-0.4178298683\c,3.5635720239,-0.0214055563,0.6597198
001\c,4.3349932998,-2.2206146679,-0.2743464828\c,4.7701224657,0.842129
3375,0.3918770805\h,3.4915067114,-0.6412228342,-1.4147020933\h,3.74377
98149,-0.5121119662,1.6218201274\c,1.6902084149,-2.4090035717,0.975047
0233\c,2.2939622663,2.1171278526,0.0248735048\c,1.2728289028,-2.131394
183,-1.4745913175\c,1.7754338276,0.9551133724,2.1801274205\h,2.1894102
987,-2.039215935,1.8746892242\h,2.6224567244,1.9974063784,-1.012870686
4\h,2.097686432,-3.4011133414,0.7498783856\h,2.9920373125,2.7801232121
,0.5478882568\h,0.6249946801,-2.5158888778,1.1936649275\h,1.3120462295
,2.5975232178,0.0192392999\h,1.3760875027,-1.4699099786,-2.3404309333\
h,1.5945600085,0.0000721808,2.6813923752\h,1.762377233,-3.0836359667,-
1.6959266735\h,2.5670671396,1.4903489793,2.715498362\h,0.2073667257,-2
.3272479409,-1.3051710377\h,0.8575551103,1.5464803219,2.2300452653\o,5
.1204866764,1.5593480019,1.4784580972\o,5.3698820954,0.9127697449,-0.6
530735373\h,5.8979827556,2.0929145137,1.2359566299\o,4.2654881451,-3.0
820203964,-1.3087692459\o,5.0924494519,-2.3826307902,0.651588681\h,4.9
235993084,-3.7813009179,-1.1469111784\c,-1.0042440453,0.1635531233,-0.
3972657179\c,-2.2796435557,-0.4928849695,0.1278714642\c,-1.0944079225,
1.6699350948,-0.491721673\h,-0.7508725312,-0.2350471321,-1.386266249\c
,-0.8503540166,2.3219617161,-1.6996051543\c,-0.8890599318,3.7149266907
,-1.7776580518\c,-1.1704871375,4.4669191379,-0.6396269864\c,-1.4209360
914,3.8218446332,0.5738513478\c,-1.3868450878,2.4322151462,0.644460224
8\h,-0.6011761779,1.734373143,-2.5808916657\h,-0.6872641567,4.21060161
68,-2.7228092916\h,-1.1931411115,5.5513918549,-0.6941986087\h,-1.63906
91262,4.404629388,1.4642913492\h,-1.5683801502,1.9317983097,1.59324084
84\c,-3.545383626,-0.1478184012,-0.6741690362\h,-2.125749896,-1.580750
7683,0.1245240224\h,-2.4216100355,-0.2009607035,1.1761726231\c,-4.7541
580241,-0.7927271102,-0.0227720146\h,-3.6890692747,0.9397936091,-0.624
0887101\c,-3.4096338213,-0.5367274053,-2.1519828205\c,-5.678467249,-0.
0166422807,0.681248814\c,-6.7818941993,-0.6003336636,1.3035760187\c,-6
.9769538712,-1.9775129572,1.2301587692\c,-6.0612341452,-2.7642181702,0
.5314198765\c,-4.9610065262,-2.1756024616,-0.0875113195\h,-5.531681061
,1.05994909,0.7403118976\h,-7.4893662229,0.0226634921,1.8435721522\h,-
7.8357919423,-2.4356428157,1.7118309307\h,-6.2047188275,-3.8392557264,
0.4680326798\h,-4.2555639352,-2.8024393242,-0.6287857523\h,-4.36360112
33,-0.4148773103,-2.6735836129\h,-2.6677182525,0.0908130257,-2.6564758
468\h,-3.0940261804,-1.5813571275,-2.2620035839\Version=EM64L-G09RevC
.01\HF=-1440.9473004\RMSD=8.666e-09\RMSF=1.073e-06\Dipole=-0.6914146,0
.2069865,-0.0815593\Quadrupole=-9.4378821,12.3231506,-2.8852685,0.6714
992,-1.944655,4.9616069\PG=C01 [X(C26H33N1O5)]\@\n

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**13-P**

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1\1\GINC-D18\FOpt\RM062X\Gen\C10H15N1O5\ETS502\30-May-2013\0\#M062X/g
en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdisk=214
7483648\sty_phehe_core.freq\0,1\N,1.521250999,-0.2619243059,0.017245
9254\o,0.2052017896,-0.5144380345,0.4559467518\c,2.0774790469,-1.50165
55099,-0.5309090226\c,2.366049862,0.0282643749,1.1772012278\c,3.598887
7743,-1.2339504137,-0.4794521156\c,3.764845991,-0.113106587,0.56695111
07\c,4.3589939446,-2.4860922036,-0.1203203435\c,4.250322644,1.17000108
24,-0.0780330352\h,3.961774663,-0.8925077685,-1.4539989219\h,4.5030060
724,-0.3891641449,1.3280561793\h,1.7981753473,-2.350165039,0.113631326
5\h,2.1500457064,1.0183979572,1.5812036459\h,1.7047887239,-1.686844052
3,-1.5397276251\h,2.2113446323,-0.7267443371,1.9639200419\o,4.14719917

```

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44,2.2189499467,0.761870833\O,4.7110944616,1.2766594763,-1.187846607\H
,4.5065258489,2.9962030535,0.2989491041\O,4.1456054272,-3.4577214152,-
1.0289103427\O,5.0630019462,-2.6442941941,0.8469127998\H,4.6484303128,
-4.2415562181,-0.7450694957\C,-0.7242899303,0.3369706542,-0.2328883135
\C,-2.0997422564,-0.1823758266,0.1396188727\C,-0.4700258997,1.78186723
29,0.1163058016\H,-0.5536841396,0.2039990357,-1.311877906\C,-1.3722793
922,2.6374625731,0.5933053329\H,-2.4035135707,2.3508713696,0.781718191
1\H,-2.8759864642,0.3631075821,-0.4041300954\H,-2.1744594004,-1.241982
1971,-0.1169819802\H,-2.2744902411,-0.0713015973,1.2140143496\H,-1.106
961373,3.6675640219,0.8117661895\H,0.5504992999,2.1165404845,-0.066605
8794\"Version=EM64L-G09RevC.01\HF=-820.6025891\RMSD=6.532e-09\RMSF=3.6
88e-06\Di pole=-0.4938938,0.0485452,-0.064865\Quadrupole=-4.5887681,9.4
224519,-4.8336838,-0.0213542,0.4527676,4.743922\PG=C01 [X(C10H15N1O5) ]
\\@
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**13<sup>-</sup>P (core)**

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1\1\GINC-D12\FOpt\RM062X\Gen\C26H32N1O5(1-)\ETS502\26-Jun-2013\0\\#M06
2X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdisk
=3489660928\sty_phece_mo62x.freq\|-1,1\N,1.056211,-0.053591,0.318396\
0,0.075748,0.29417,1.284488\C,2.172584,0.938728,0.271572\C,1.5748,-1.4
23772,0.576107\C,3.415293,0.013925,0.070278\C,2.865453,-1.373452,-0.25
37\C,4.377386,0.514049,-0.97038\C,3.896012,-2.51193,0.035035\H,3.98199
5,-0.044765,1.003596\H,2.599684,-1.421657,-1.318528\C,1.92298,1.878318
,-0.912739\C,1.869068,-1.712659,2.05498\C,2.319824,1.768187,1.550133\C
,0.569548,-2.44756,0.058312\H,1.840836,1.308343,-1.842604\H,2.656438,-
1.06659,2.455097\H,2.742622,2.601329,-1.013833\H,2.215668,-2.747049,2.
136904\H,0.992424,2.435173,-0.758807\H,0.967035,-1.576875,2.660896\H,2.
368787,1.131378,2.437744\H,0.286355,-2.213417,-0.974398\H,3.246871,2.
349469,1.485312\H,1.034765,-3.436923,0.087301\H,1.478724,2.459037,1.66
7501\H,-0.337752,-2.447814,0.680441\O,5.072178,-2.126688,0.223276\O,3.
425146,-3.672563,0.036992\O,5.301695,1.360282,-0.446139\O,4.34833,0.28
5068,-2.15658\H,5.884099,1.609715,-1.183607\C,-1.210542,0.358731,0.681
425\C,-2.205695,-0.00686,1.782366\C,-1.476918,1.726576,0.086971\H,-1.2
55648,-0.386328,-0.120488\C,-1.858538,1.86521,-1.247202\C,-2.085711,3.
129432,-1.793558\C,-1.928749,4.268258,-1.006338\C,-1.5452,4.137817,0.3
30372\C,-1.324009,2.874362,0.87154\H,-1.959808,0.974898,-1.86417\H,-2.
369567,3.223854,-2.838337\H,-2.093514,5.254174,-1.432587\H,-1.408998,5
.02311,0.945942\H,-0.99946,2.769569,1.904762\H,-2.06869,0.680456,2.628
149\C,-3.676238,0.033333,1.343791\H,-1.939026,-1.00699,2.149638\H,-3.9
26548,1.075928,1.104044\C,-3.942845,-0.789811,0.096528\C,-4.585013,-0.
423053,2.493019\H,-5.640714,-0.353133,2.210713\H,-4.375178,-1.465949,2
.757717\H,-4.420845,0.192988,3.384408\C,-3.497463,-2.112811,-0.008277\
C,-3.743226,-2.862665,-1.155786\C,-4.452198,-2.304207,-2.219616\C,-4.9
08131,-0.991049,-2.125604\C,-4.65093,-0.242773,-0.976733\H,-2.929233,-
2.558129,0.805544\H,-3.367287,-3.879575,-1.223908\H,-4.636837,-2.88581
9,-3.118325\H,-5.453321,-0.542228,-2.951763\H,-4.984621,0.791544,-0.91
7438\"Version=EM64L-G09RevC.01\HF=-1440.4087196\RMSD=9.363e-09\RMSF=3.
546e-06\Di pole=-6.8159663,4.2894426,0.226762\Quadrupole=-35.0051579,4.
9026005,30.1025574,35.809772,2.9612947,0.6317471\PG=C01 [X(C26H32N1O5)
]\\@
```

**13<sup>-</sup>P**

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1\1\GINC-V1267\FOpt\RM062X\Gen\C10H14N1O5(1-)\ETS502\01-Jul-2013\0\\#M
062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdi
sk=268435456\sty_phece_core.freq\|-1,1\C,0.897884761,-0.2166126464,0.
3853633924\C,-0.071552477,0.3149122474,1.4264510811\C,0.6834968407,1.5
532611751,1.9350237006\C,2.1515494644,1.0824382759,1.9493367307\N,2.20
47943457,-0.1073137516,1.0578207406\O,3.2049741952,0.0826550025,0.0614
375737\C,-1.5051517194,0.6505218296,0.9298446202\O,-1.9118391295,-0.00
40351686,-0.0543343412\O,-2.0792538303,1.5369530051,1.6063613283\C,0.1
938787956,2.0029754437,3.2821095583\O,0.1119113583,1.3019759606,4.2666
533689\O,-0.0831818498,3.3239879506,3.3336997954\C,4.291892211,-0.7995
817363,0.2946966475\C,5.1541276973,-0.7380678736,-0.9596339158\C,5.240
1709749,-1.1566812674,2.5912688729\C,5.0695320103,-0.3884499531,1.5176
278465\H,5.8087933154,-0.8209674303,3.4540795673\H,5.4944293835,0.6170
58598,1.4831663876\H,0.5389404099,2.3714427191,1.2238335925\H,-0.15487
36732,-0.4008865421,2.2561838864\H,2.4658811403,0.7839025366,2.9554922
813\H,0.8732882299,0.4161694946,-0.5140246088\H,2.8408709644,1.8460846
121,1.5729740524\H,0.7009429882,-1.2492053142,0.0906857357\H,-0.469690
8324,3.4834785614,4.2111496269\H,3.8965085215,-1.8142007841,0.44290151
76\H,4.7900669771,-2.1454073369,2.6480057934\H,5.5329775012,0.27897348
31,-1.1081028517\H,6.0059806404,-1.4191935862,-0.8698121771\H,4.560133
```

7853,-1.0150635042,-1.8352438041\\Version=EM64L-G09RevC.01\HF=-820.059  
 6749\RMSD=6.750e-09\RMSF=3.175e-06\Di pole=5.5259557,-0.1937836,0.71174  
 01\Quadrupole=-8.3020988,9.5859231,-1.2838243,5.2976663,2.5811071,-2.3  
 660675\PG=C01 [X(C10H14N1O5)]\\@

### **13<sup>2-</sup>-P (core)**

1\\1\GINC-D22\FOpt\RM062X\Gen\C26H31N1O5(2-) \ETS502\13-Aug-2013\0\\#M06  
 2X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdisk  
 =3489660928\\sty\_pcece\_unfinished.freq\\-2,1\N,-1.0082533052,-0.227677  
 9512,0.0667237436\O,-0.0956401868,-1.301475053,-0.1964282169\C,-2.1285  
 653811,-0.7269934583,0.9095367485\C,-1.5546182865,0.358117121,-1.21248  
 07239\C,-3.2239193816,0.3201703311,0.5952241181\C,-3.0727510004,0.5732  
 907875,-0.9044860196\C,-4.6067705922,-0.2247404844,1.0848318178\C,-3.5  
 313709751,1.9604271744,-1.4531813278\H,-3.0051979468,1.2432994951,1.14  
 57200035\H,-3.6539494141,-0.1846473495,-1.4404353853\C,-2.5821598965,-  
 2.1462333289,0.5278968325\C,-0.8158638918,1.6805794338,-1.4655160119\C  
 ,-1.7200783937,-0.7167779363,2.3799915379\C,-1.3682926013,-0.546937711  
 8,-2.4311623181\H,-2.9766869188,-2.1828376571,-0.4908875864\H,-0.96115  
 47816,2.3572765447,-0.6170041846\H,-3.394162016,-2.4458288259,1.198059  
 1653\H,-1.2263749976,2.1675415015,-2.3560396416\H,-1.752260345,-2.8565  
 329863,0.6241553203\H,0.2585439395,1.507306992,-1.6165324153\H,-1.3344  
 149735,0.2727140523,2.6553153267\H,-1.7812037709,-1.5450671449,-2.2569  
 980353\H,-2.6091219545,-0.9138225073,2.9867009968\H,-1.912665024,-0.07  
 86615254,-3.2588384623\H,-0.9480320114,-1.4734790285,2.584446317\H,-0.  
 3094915476,-0.6574228604,-2.7049814137\O,-3.5876735243,2.9162366005,-0  
 .6456114475\O,-3.7094802115,1.9903582812,-2.70183073\O,-4.7709873416,-  
 0.1879675346,2.3357053068\O,-5.3713148671,-0.7151483561,0.2247007752\C  
 ,1.2406443334,-0.8598459142,-0.0712449997\C,1.5747333025,-0.5767386306  
 ,1.4008554404\C,2.1318744854,-1.9410703516,-0.639810843\H,1.3830320712  
 ,0.0532835389,-0.663350905\C,3.382248849,-1.6171556698,-1.1753723591\C  
 ,4.2338365637,-2.6132706408,-1.6521650127\C,3.8389793724,-3.9499988862  
 ,-1.6070876542\C,2.5865610735,-4.278799583,-1.0868462699\C,1.738273496  
 8,-3.2827484455,-0.606028647\H,3.681635071,-0.5710235889,-1.2283409874  
 \H,5.2007531138,-2.3432662613,-2.0702157803\H,4.4969952961,-4.72860956  
 08,-1.9854268916\H,2.2642606601,-5.3169886945,-1.0630828811\H,0.752942  
 3954,-3.5249071639,-0.2179030352\H,0.7428026979,0.013514757,1.79727162  
 43\H,1.5680768435,-1.5329552857,1.9421666119\C,2.9021213103,0.13929367  
 79,1.6643462054\C,3.0817764407,0.3491240235,3.1766733357\H,3.727480787  
 3,-0.5000851487,1.3166252757\C,3.0287081522,1.4755717514,0.9514954731\  
 H,4.0413364113,0.8298493912,3.3997273391\H,2.2813216715,0.9895890277,3  
 .5642215652\H,3.0381614715,-0.609169162,3.7071247255\C,4.295743591,1.9  
 555726057,0.598428767\C,4.451652115,3.1969634811,-0.015813397\C,3.3311  
 474937,3.9799027692,-0.2953166133\C,2.0631335917,3.5097191444,0.042667  
 8418\C,1.9133083879,2.2711660532,0.6659362015\H,5.1702082154,1.3379758  
 554,0.8032952747\H,5.4452016005,3.5465096743,-0.2874660996\H,3.4437996  
 922,4.9414715936,-0.7893316075\H,1.1761170829,4.0896001422,-0.19762039  
 4\H,0.9096929584,1.9101848854,0.8846696065\\Version=EM64L-G09RevC.01\HF  
 =-1439.7592964\RMSD=6.545e-09\RMSF=5.019e-06\Di pole=13.067905,-2.7057  
 616,0.6482962\Quadrupole=-69.7223657,36.6961591,33.0262066,21.0351306,  
 -0.6188323,10.5556246\PG=C01 [X(C26H31N1O5)]\\@

### **13<sup>2-</sup>-P**

1\\1\GINC-D16\FOpt\RM062X\Gen\C10H13N1O5(2-) \ETS502\26-Jun-2013\0\\#M06  
 2X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) Nosymm maxdisk  
 =2147483648\\sty\_pcece\_core.freq\\-2,1\N,-0.944403851,-0.3172396652,0.  
 1854234154\C,0.0627099771,-1.3464668535,0.4757024464\C,-0.796540966,-2  
 .6079893195,0.4353916097\C,-2.1042078927,-2.1641418786,1.1263259535\C,  
 -2.0492662212,-0.6178940972,1.1069007574\C,-2.3276399834,-2.6424439044  
 ,2.5962518585\O,-1.5005743385,-3.4420222655,3.0969806803\O,-3.34657873  
 13,-2.1446695656,3.1508415676\C,-0.9359542868,-3.1390753054,-1.0355326  
 769\O,0.1410731214,-3.1677301255,-1.6932893702\O,-2.0692653703,-3.5180  
 936497,-1.4149542322\O,-0.4171078794,0.9806739085,0.5037399279\C,-0.23  
 80830554,1.6878766753,-0.698626606\C,-1.5838227926,2.0379666155,-1.339  
 0600599\C,0.5622290518,2.9290877527,-0.4161141653\C,1.0178231824,3.294  
 1420134,0.7822921464\H,0.83407247,2.6708090326,1.6518798725\H,1.583799  
 8728,4.2136693055,0.9147151898\H,0.7501567786,3.5607992619,-1.28695546  
 31\H,-2.9466665833,-2.5246528885,0.5287287092\H,-0.3344116788,-3.40379  
 34613,1.0292934514\H,-1.8138941069,-0.2248267754,2.1081526089\H,0.8491  
 270079,-1.3498347719,-0.2826473971\H,-2.9709471855,-0.1380970741,0.759  
 5203208\H,0.4865595494,-1.1738295565,1.4816057618\H,0.3262367915,1.054  
 6970678,-1.4038816768\H,-2.1309413809,1.1089532189,-1.5186140091\H,-2.  
 1608569205,2.6746541229,-0.6586400113\H,-1.4434115784,2.5652431827,-2.

2914416097\\Version=EM64L-G09RevC.01\\HF=-819.4106617\\RMSD=4.042e-09\\RM  
SF=7.199e-06\\Dipole=2.0164501,6.6292154,-1.3828522\\Quadrupole=16.53627  
5,-18.766204,2.2299289,-30.6608692,23.1611955,8.9858595\\PG=C01 [X(C10H  
13N1O5)]\\@

**16 (core)**

```
1\\1\GINC-R2830\FOpt\UM062X\Gen\C6H10N1O3(2) \ROOT\13-Aug-2014\0\\#M062X
/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=53687091
2\\apyrh_rcore.freq\\0,2\N,-0.9558922404,-0.5797294869,0.3708427592\O,
-1.060578922,-1.6017126871,1.1100111435\C,0.3048462666,0.1610852029,0.
2166794704\O,C,-2.1093038639,0.0875543571,-0.2407120633\O,C,-0.0406799032,
1.1523192542,-0.8938402177\O,C,-1.5350243277,1.4419024259,-0.6644669928\
H,0.1048034828,0.671574696,-1.8703263773\H,-1.6509168757,2.1667965414,
0.1482533688\O,C,1.439625747,-0.8070650892,-0.072009662\H,1.2781737303,-
1.328273707,-1.0233760835\O,C,2.7714303416,-0.1066123493,-0.1192252572\H
,1.4754992396,-1.5819102571,0.7027249635\H,0.5850312684,2.0454070294,-
0.8545566702\H,-2.0269884983,1.8475764448,-1.5512331467\O,2.9629898946
,1.062144301,0.1188591089\O,O,3.766174665,-0.9469580648,-0.4623102924\H,
4.5939549436,-0.4343870558,-0.4607639385\H,0.5161348501,0.6953770115,1
.1548950812\H,-2.4591659182,-0.5084621768,-1.0931617835\H,-2.915843880
2,0.1478136099,0.4950165896\\Version=EM64L-G09RevC.01\\State=2-A\\HF=-51
4.8280489\\S2=0.755242\\S2-1=0.\\S2A=0.750018\\RMSD=8.776e-09\\RMSF=6.676e-
06\\Dipole=0.0649017,0.6989157,-0.9183039\\Quadrupole=5.7111511,-5.25352
92,-0.4576219,-6.1239358,2.0327109,1.8341094\\PG=C01 [X(C6H10N1O3)]\\@
```

**16**

```
1\\1\GINC-R2503\FOpt\UM062X\Gen\C9H16N1O3(2) \ROOT\13-Aug-2014\0\\#M062X
/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=80530636
8\\apyrh_r.freq\\0,2\N,-0.0696991402,-0.089123986,1.7459536873\O,-0.13
62559999,-0.1074406473,3.0110710704\O,C,-0.5446498722,1.064023304,0.9501
386529\O,C,0.4915824652,-1.2122412918,0.9625159713\O,C,0.0164031644,0.7263
927691,-0.4402057712\O,C,0.0887993024,-0.8095516782,-0.4635212067\H,1.01
94242428,1.1566824146,-0.5514338146\H,-0.8944962342,-1.2315650744,-0.7
025492502\O,C,-2.076086136,1.0894938053,0.9846154621\O,C,2.0113994112,-1.2
36891303,1.1576035057\O,C,0.0490853233,2.327769592,1.5740337376\O,C,-0.133
3276691,-2.5220766982,1.4299919821\H,-2.4832865532,0.1829221797,0.5247
386755\H,2.4753606261,-0.3244202589,0.7672334621\H,-2.4552571872,1.957
4990907,0.4389398724\H,2.4461442106,-2.096506538,0.636605539\H,-2.4192
982368,1.1292538563,2.0232503976\H,2.2449938922,-1.3152844187,2.223741
1777\H,1.1363559369,2.2195152053,1.6809446445\H,-1.2241142406,-2.47911
27239,1.3467308248\O,C,-0.2045694046,3.5804386901,0.775759317\H,0.234067
1717,-3.3504561721,0.8151958483\H,-0.3387920356,2.4671180178,2.5893820
062\H,0.1251108889,-2.7141453771,2.4750205604\H,-0.6067568174,1.139341
1746,-1.2355583816\H,0.7998580215,-1.1831966789,-1.2062701181\O,-0.753
067614,3.6527875586,-0.2983692821\O,O,0.2834120366,4.667532439,1.4057059
948\H,0.1003304474,5.4373427498,0.8385054347\\Version=EM64L-G09RevC.01
\\State=2-A\\HF=-632.7244622\\S2=0.755267\\S2-1=0.\\S2A=0.750018\\RMSD=6.660
e-09\\RMSF=1.032e-05\\Dipole=0.3352299,-0.015712,-0.8518683\\Quadrupole=0
.8520856,6.4629285,-7.3150141,0.1782875,-1.5066375,3.841087\\PG=C01 [X(
C9H16N1O3)]\\@
```

**16-P (core)**

```
1\\1\GINC-R489\FOpt\RM062X\Gen\C10H17N1O3\ROOT\15-Aug-2014\0\\#M062X/ge
n 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=805306368\\
psapyrh_core.freq\\0,1\N,-1.7476200152,-1.1179885842,0.3486648783\O,-0
.5785691897,-0.7062107379,-0.3334751576\O,C,-1.8294465067,-2.5822312611,
0.3099618302\O,C,-2.9168134282,-0.6760606565,-0.4168979534\O,C,-3.30285037
98,-2.842151091,0.6432727523\O,C,-4.0310647488,-1.5576248374,0.161874685
7\H,-3.4381663442,-2.9780323754,1.718938455\H,-4.8000713432,-1.7606453
468,-0.5881807614\O,C,-3.1456201369,0.8239491787,-0.2563713742\H,-3.2012
260552,1.0845942087,0.8028886607\O,C,-4.4220862937,1.2658505756,-0.92115
27276\H,-2.3084039335,1.3658479131,-0.7110832729\O,C,0.3836944949,-0.190
7793795,0.5940897564\O,C,1.7005824751,-0.1515829652,-0.1658617539\O,C,-0.0
165336166,1.1705145285,1.0912103679\H,0.4509744631,-0.8837637937,1.444
1773654\O,C,-0.3205042287,1.4421539348,2.3580683377\H,-0.3102646453,0.66
25707928,3.1167073033\H,1.9655832544,-1.1514101034,-0.5203325665\H,1.6
157906716,0.5117256169,-1.0329102658\H,-3.6692934802,-3.7431629332,0.1
460545182\H,-4.5137446581,-1.0474566012,1.0019926858\O,-5.3420705651,1
.8337522078,-0.3849003622\O,-4.4480279937,0.9418434223,-2.2343109797\H
,-5.29731596,1.2570471477,-2.5903741332\H,-1.1268741324,-3.0204928011,
1.0238968348\H,-1.5749473387,-2.938870632,-0.7004851182\H,-2.759935662
8,-0.9101893844,-1.4829524618\H,-0.0414573047,1.9578300305,0.335414429
2\H,-0.594610761,2.4424312524,2.6806724553\H,2.4981633632,0.2231526741
```

```
, 0.481793572\Version=EM64L-G09RevC.01\State=1-A\HF=-671.3872068\RMSD=
3.999e-09\RMSF=1.963e-06\Di pole=0.4138645,-0.621496,-0.1112514\Quadrupole=-2.3681729,0.7069746,1.6611983,4.2875115,4.9767697,-2.3589357\PG=C01 [X(C10H17N1O3)]\\@
```

**16-P**

```
1\1\GINC-R3118\FOpt\RM062X\Gen\C25H33N1O3\ROOT\15-Aug-2014\0\\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1879048192\\psapyrh.freq\0,1\N,-1.2842259026,-0.1617535877,0.0871150607\0,0.0007427297,-0.2892727457,-0.4839470252\c,-1.8690435011,-1.505171956,0.3250521468\c,-2.2064044274,0.65072339,-0.7670694735\c,-3.3419827266,-1.1197008352,0.4735098727\c,-3.5549794438,-0.1027119444,-0.6533266672\h,-3.5012223504,-0.6528904348,1.4532648259\h,-3.7694180634,-0.6185392972,-1.5955275669\c,-1.6610540608,-2.4873680368,-0.8367034541\c,-2.299826777,2.0529104911,-0.110840696\c,-1.2754113289,-2.096879105,1.6001887244\c,-1.741143125,0.7792126654,-2.2180436877\h,-2.1512043133,-2.1539929281,-1.7555276102\h,-2.7126453933,1.9393637796,0.8959774855\h,-2.0798672972,-3.463293717,-0.567390546\c,-3.1951338484,2.9854792872,-0.8839549758\h,-0.5953181581,-2.6130683226,-1.0457843207\h,-1.3018715449,2.4891517355,-0.0409084654\h,-1.3608905946,-1.3849742414,2.427501051\h,-1.5074682579,-0.2006879938,-2.6420189459\h,-1.8005322651,-3.0193978847,1.8721780776\h,-2.5386958594,1.2341375069,-2.8164354428\h,-0.2168013323,-2.3464606495,1.4581467262\h,-0.8514487463,1.4095232372,-2.2964173509\c,1.0163361622,0.1468433882,0.4264580856\c,2.3101876328,-0.4663543576,-0.1053818925\c,1.0546556378,1.6556071568,0.5218614707\h,0.7834636728,-0.2600723253,1.4175174546\c,0.7853603809,2.2977678009,1.7298002612\c,0.7553265976,3.6913288681,1.8044203482\c,0.9906958265,4.4532634135,0.6624070308\c,1.2680779077,3.8184344727,-0.5504294395\c,1.3054432045,2.4288466757,-0.6171132594\h,0.5689056114,1.7004714779,2.613303765\h,0.5338402104,4.1790757469,2.7493993372\h,0.9541219012,5.5375084316,0.7129080224\h,1.4439111616,4.4086606845,-1.4450394765\h,1.5031030402,1.9357232502,-1.5663876977\c,3.5674089965,-0.0781043326,0.6900726923\h,2.192162732,-1.5585702176,-0.1019916129\h,2.4366631141,-0.1690952236,-1.1541089841\c,4.7966094668,-0.6742592588,0.0305109587\h,3.6700653375,1.0143268511,0.64380846\c,3.4569548859,-0.4776302869,2.1672153848\c,5.7011392625,0.1424779964,-0.6527693163\c,6.824921663,-0.3957364233,-1.279705201\c,7.0605433074,-1.7676675657,-1.2320534876\c,6.1648004628,-2.594859098,-0.5543778906\c,5.0442712061,-2.0515018832,0.0694012633\h,5.5224949551,1.215119331,-0.6920428492\h,7.5162470206,0.2585908219,-1.8033314319\h,7.9351722138,-2.1905498421,-1.7175548187\h,6.339767874,-3.6662593793,-0.5114409585\h,4.3546685346,-2.7094690682,0.5939507376\h,4.4079904175,-0.3169543285,2.6837168667\h,2.6918468159,0.1156112539,2.6786035\h,3.1872946174,-1.5352932042,2.2744713834\h,-4.0039662395,-1.988007159,0.3990084955\h,-4.3856216727,0.5812214136,-0.4626793265\o,-4.4041363414,3.0024986548,-0.8414020613\o,-2.5030894549,3.8241732838,-1.6857703341\h,-3.1575785345,4.3687425589,-2.1582552225\Version=EM64L-G09RevC.01\State=1-A\HF=-1252.4310125\RMSD=4.249e-09\RMSF=2.050e-06\Di pole=0.4745292,-0.0283264,0.0531162\Quadrupole=-11.2472454,8.7546745,2.4925709,3.9035878,-1.8388293,-3.1142167\PG=C01 [X(C25H33N1O3)]\\@
```

**16<sup>-</sup> (core)**

```
1\1\GINC-R117\FOpt\UM062X\Gen\C6H9N1O3(1-,2)\ROOT\14-Aug-2014\0\\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=536870912\\apyrc_rcore.freq\\\-1,2\N,-0.9533968722,-0.6181308546,0.3399642444\0,-1.1605757942,-1.6600975246,1.0333730551\c,0.3484373432,0.0844325601,0.2686548805\c,-2.0578599246,0.1250582859,-0.2690301533\c,0.04905359,1.1851494823,-0.748235317\c,-1.441731609,1.4990196424,-0.5420397475\h,0.2165277164,0.7919225322,-1.7607270819\h,-1.5681441714,2.1413218993,0.3376982604\c,1.4978037486,-0.8325159277,-0.1049741871\h,1.303789533,-1.3015306607,-1.0784303502\c,2.868528917,-0.0804503302,-0.165438947\h,1.5777894162,-1.6438190569,0.6275804529\h,0.7165193969,2.0342538281,-0.5995151424\h,-1.9011295433,2.0034408449,-1.3977100409\o,2.8817392993,1.0763692406,0.3255646615\o,3.7990965148,-0.7284987411,-0.689543327\h,0.551975688,0.5308474447,1.2522793018\h,-2.3726690993,-0.3804013863,-1.1936600184\h,-2.9051741496,0.1317387217,0.4245794562\Version=EM64L-G09RevC.01\State=2-A\HF=-514.2818717\S2=0.755418\S2-1=0.\S2A=0.75002\RM SD=8.120e-09\RMSF=3.397e-06\Di pole=-4.3325575,0.9472281,-0.4866184\Quadrupole=-18.3315199,5.9540539,12.377466,-4.7559147,5.3973149,0.6372976\PG=C01 [X(C6H9N1O3)]\\@
```

**16<sup>-</sup>**

```
1\1\GINC-R117\FOpt\UM062X\Gen\C9H15N1O3(1-,2)\ROOT\14-Aug-2014\0\\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=805306
```

```

368\\apyrc_r.freq\\-1,2\\N,-1.0091545681,-0.5264737774,0.5001126048\\O,-
1.1772606853,-1.5735736036,1.1976303541\\C,0.2900206309,0.1992454542,0.
4062585702\\C,-2.1072507503,0.0350530357,-0.3106229002\\C,-0.0167309325,
1.212664184,-0.709144087\\C,-1.5395015458,1.4143842989,-0.6681662358\\H,
0.2928760069,0.793151132,-1.6738239613\\H,-1.8091470484,2.1317775856,0.
117978679\\C,0.5553543238,0.8770118837,1.7531478572\\C,-2.3140667306,-0.
8491580022,-1.54677956\\C,1.408739643,-0.7747649472,0.0393578393\\C,-3.3
836516,0.0940523924,0.5220856886\\H,-0.2238443361,1.6161300144,1.983222
5948\\H,-1.4200777334,-0.8500940845,-2.1787974335\\H,1.5287069114,1.3708
842182,1.6994060167\\H,-3.1634773933,-0.4874271201,-2.1389757682\\H,0.56
01174317,0.12181497,2.5467332131\\H,-2.5130430745,-1.8784691528,-1.2308
830432\\H,1.0938865294,-1.3722019356,-0.8270346614\\H,-3.2150604015,0.67
53371436,1.4348937671\\C,2.7860945378,-0.1185159628,-0.3171581324\\H,-4.
1862100945,0.56757707,-0.0557188833\\H,1.5623974026,-1.4852600632,0.859
8765184\\H,-3.6965503912,-0.9138400281,0.8105080572\\H,0.5577755216,2.12
83292055,-0.5666500294\\H,-1.9475827989,1.787996745,-1.6142902993\\O,2.8
600554713,1.1332472444,-0.2338348444\\O,3.6647756742,-0.9387179,-0.6564
719211\\Version=EM64L-G09RevC.01\\State=2-A\\HF=-632.1784237\\S2=0.755398
\\S2-1=0.\\S2A=0.75002\\RMSD=7.744e-09\\RMSF=1.259e-05\\Dipole=-5.1312468,0
.903264,-0.0091048\\Quadrupole=-24.3824711,9.0628632,15.3196079,-1.4859
282,8.5601778,1.8339329\\PG=C01 [X(C9H15N1O3)]\\@
```

**16<sup>-</sup>P (core)**

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1\\1\\GINC-R118\\FOpt\\RM062X\\Gen\\C10H16N1O3(1-)\\ROOT\\16-Aug-2014\\0\\#M062
X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=8053063
68\\psapycrc_core.freq\\-1,1\\N,-1.8006594313,-1.1000642743,0.3521800909
\\O,-0.6074084382,-0.741315085,-0.3313819853\\C,-1.8561774228,-2.5587208
464,0.4597371305\\C,-2.9594025695,-0.7541471794,-0.5024824619\\C,-3.3367
267888,-2.8103526565,0.7742684841\\C,-4.0653971382,-1.5863353402,0.1548
398746\\H,-3.4968292953,-2.85784377,1.8560425401\\H,-4.8216310867,-1.841
2196758,-0.5874729963\\C,-3.2349540181,0.7329004574,-0.5742727865\\H,-3.
3742261298,1.1361787646,0.4377698995\\C,-4.4812577458,1.1047382473,-1.4
429017471\\H,-2.3710270876,1.2508389122,-1.0113915059\\C,0.3331712068,-0
.1920634462,0.5752234715\\C,1.5566489646,0.1408288066,-0.2726419289\\C,-
0.197120347,1.0328412507,1.2720331592\\H,0.6007758414,-0.9481162754,1.3
325791753\\C,0.0339629327,1.3148639924,2.5523116569\\H,0.5787452151,0.62
3282941,3.1936194694\\H,1.8988720615,-0.751899113,-0.8052977737\\H,1.298
8450205,0.9071396254,-1.0109433938\\H,-3.672363211,-3.7613174705,0.3491
833963\\H,-4.5538811875,-0.9907597247,0.9343090726\\O,-4.8234665851,2.30
61296159,-1.3757774607\\O,-4.9854793915,0.1719135065,-2.1156708247\\H,-1
.1664196528,-2.9175060754,1.232094164\\H,-1.5707288973,-3.0113678232,-0
.504786268\\H,-2.7742735274,-1.1385062128,-1.5196307089\\H,2.364624207,0
.5185832411,0.3607147723\\H,-0.7706463897,1.713743019,0.6433676199\\H,-0
.3279591083,2.2308625885,3.0095978646\\Version=EM64L-G09RevC.01\\State=
1-A\\HF=-670.8356833\\RMSD=3.587e-09\\RMSF=3.295e-06\\Dipole=4.4385527,-2.
5837921,2.8786278\\Quadrupole=-10.5952962,4.8513703,5.7439259,14.476583
4,-17.4262853,7.0592596\\PG=C01 [X(C10H16N1O3)]\\@
```

**16<sup>-</sup>P**

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1\\1\\GINC-R118\\FOpt\\RM062X\\Gen\\C25H32N1O3(1-)\\ROOT\\17-Aug-2014\\0\\#M062
X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1879048
192\\psapycrc.freq\\-1,1\\N,-1.654863128,-1.1674366373,0.2512461124\\O,-0
.3780000815,-0.9802461853,-0.3396085387\\C,-1.8870189056,-2.6132679417,
0.4595113768\\C,-2.7788744139,-0.5760809911,-0.5778485894\\C,-3.41007741
79,-2.6113953966,0.6132512595\\C,-3.8754950685,-1.6668400036,-0.4989775
083\\H,-3.673612109,-2.2057626496,1.5984447277\\H,-3.9382452051,-2.20792
28235,-1.4515471854\\C,-1.4490731728,-3.495953194,-0.7202105009\\C,-3.25
59377702,0.7226176005,0.0960846316\\C,-1.1586490071,-3.0705285641,1.722
1832276\\C,-2.3709621946,-0.3013005912,-2.0256509612\\H,-1.9899358801,-3
.2480100415,-1.6369614811\\H,-3.6806580962,0.4616313286,1.0755783671\\H,
-1.6441921075,-4.5489575488,-0.4819144882\\C,-4.3151220548,1.4748630745
,-0.7639068087\\H,-0.3791931143,-3.3744078329,-0.9135991747\\H,-2.401512
5096,1.3832731358,0.2520614305\\H,-1.4198329712,-2.4205794308,2.5639149
039\\H,-1.8950142765,-1.1757858506,-2.4831537999\\H,-1.4320754065,-4.103
4589327,1.9718337754\\H,-3.271552244,-0.040516484,-2.5904175638\\H,-0.07
06276653,-3.0383630808,1.5782356876\\H,-1.6877847588,0.5489964131,-2.08
91229002\\C,0.5022755413,-0.3011813962,0.5510591565\\C,1.8966265273,-0.5
285797466,-0.0348668819\\C,0.1448006716,1.1619864508,0.6861644901\\H,0.4
255006826,-0.7708915993,1.5406448552\\C,-0.2038497834,1.6974241447,1.92
43390622\\C,-0.629644598,3.0220676744,2.030553477\\C,-0.7234930188,3.814
8794367,0.8900636902\\C,-0.3680326102,3.2888842809,-0.3527795529\\C,0.07
93641695,1.9757700998,-0.4489654729\\H,-0.193608612,1.055829425,2.80373
```

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46548\H,-0.9288516052,3.4192261215,2.9968168185\H,-1.1075575106,4.8282
4418,0.9591392871\H,-0.4898631712,3.8869755381,-1.2502767143\H,0.31318
56805,1.5524430394,-1.4231300338\c,3.0284298564,0.1793688716,0.7302611
136\H,2.0913731762,-1.6103228195,-0.0575166902\H,1.8914876284,-0.18752
98264,-1.0779402042\c,4.3366333335,-0.027697734,-0.0093941169\H,2.8136
294351,1.2563864972,0.7148665016\c,3.084705412,-0.2656027322,2.1949566
405\c,4.7005411792,0.8582108634,-1.0301649383\c,5.871409123,0.67436845
5,-1.7617432391\c,6.7065063484,-0.4077290359,-1.4840470239\c,6.3563129
557,-1.2989229931,-0.4718316596\c,5.1822118438,-1.1092271957,0.2570516
111\H,4.049446544,1.7025202875,-1.2504607674\H,6.1329011898,1.37750662
96,-2.5479611502\H,7.6214965204,-0.5540682901,-2.0512869073\H,6.998434
238,-2.1465721053,-0.2470027716\H,4.9241323982,-1.8139278062,1.0434626
417\H,3.9907797651,0.1054977537,2.6857899288\H,2.2207316447,0.12176130
75,2.7429671761\H,3.0677823066,-1.3589714357,2.2842441336\H,-3.8289520
52,-3.6217614938,0.5367494751\H,-4.84734132,-1.1994158258,-0.322291674
8\O,-5.4588787916,0.9528309342,-0.803811405\O,-3.9045655393,2.50326267
29,-1.3525995092\Version=EM64L-G09RevC.01\State=1-A\HF=-1251.8778956\RMSD=9.543e-10\RMSF=2.793e-06\Dipole=7.2215604,-2.4557158,1.8638191\Quadrupole=-50.1603534,20.4249611,29.7353922,22.1843204,-18.4998149,4.97
90413\PG=C01 [X(C25H32N1O3)]\\@
```

**19** (core)

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1\1\GINC-R94\FOpt\UM062X\Gen\C10H12N1O3(2)\ROOT\14-Aug-2014\0\#M062X/
gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=805306368
\stnh_rcore.freq\0,2\N,-2.3844314271,-0.476820093,-0.3707149632\O,-2
.6950498818,-0.3503328122,-1.6010366827\c,-2.0355016786,-1.8086627578,
0.1056015604\c,-1.7953134049,0.6810355325,0.3048282938\c,-0.2895424976
,0.7173476607,0.1480886398\H,-2.0666300827,0.6385822318,1.3652987408\c
,0.2772758197,0.7405494299,-1.1286629722\c,1.6610934394,0.7442175131,-
1.2799376335\c,2.5046462241,0.7296584056,-0.166229115\c,1.9351983595,0
.7048165543,1.108022988\c,0.5511766539,0.6941326069,1.2618899639\H,-0.
3720366751,0.743236563,-2.0011534829\H,2.0914149172,0.7600457162,-2.27
86486147\c,4.0006635459,0.7411769548,-0.3408609955\H,2.5771942184,0.67
52447202,1.9843798103\H,0.1211297987,0.6658062067,2.2608243031\c,4.685
0952918,-0.5116572422,0.1678265724\H,4.4552476929,1.5787796089,0.20536
1275\H,4.2802217534,0.8775099269,-1.389970904\O,4.2098559417,-1.345839
9221,0.8949148833\O,5.9570707138,-0.5771023319,-0.2787802723\H,6.35638
61761,-1.3799922469,0.1003787851\H,-2.746675059,-2.5122330889,-0.32756
82579\H,-2.0939991891,-1.8318116777,1.1968081096\H,-1.017449768,-2.071
4629625,-0.2082051153\H,-2.2684208824,1.5554955036,-0.1484349162\Version=EM64L-G09RevC.01\State=2-A\HF=-668.3934819\S2=0.755156\S2-1=0.\S2A=0.750016\RMSD=2.572e-09\RMSF=1.705e-06\Dipole=0.9713924,0.1984302,0.8
06469\Quadrupole=0.4244736,0.2730911,-0.6975646,0.3288476,-8.995129,0.
5324918\PG=C01 [X(C10H12N1O3)]\\@
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**19**

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1\1\GINC-R92\FOpt\UM062X\Gen\C16H24N1O3(2)\ROOT\14-Aug-2014\0\#M062X/
gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=134217728
0\stnh_r.freq\0,2\N,-2.1252060249,-0.3117515073,-0.3568579475\O,-2.2
241598712,-0.269362333,-1.6271792991\c,-3.5949078215,-2.2353035123,-0.
2292842314\c,-1.8684838727,2.1453299103,-0.3246427052\c,-2.2698587486,
-1.6568483387,0.2738628955\c,-1.4177466791,0.8103006808,0.2948986393\c
,-1.0988018829,-2.5450506393,-0.1675038932\c,0.0841600132,0.5951061012
,0.2339797054\c,-2.303327499,-1.5357457481,1.7963878653\H,-1.345816779
5,-1.1956265308,2.2035766543\H,-2.5067995436,-2.5243730104,2.219259390
1\H,-1.2590674123,-3.5688642569,0.1876046315\H,-0.1480399354,-2.184102
5697,0.2375176595\H,-1.034452941,-2.5576883531,-1.2595666474\H,-4.4305
456013,-1.5913504534,0.0660196123\c,-1.1658322679,3.3079594959,0.37875
37688\H,-3.5882243913,-2.317288585,-1.3179777007\c,-3.3876109326,2.293
3684232,-0.23139517\H,-3.748915768,-3.2291941453,0.202692277\H,-1.5778
867608,2.1355685651,-1.3815241149\H,-3.0982956213,-0.8575814406,2.1270
601089\H,-1.7264530815,0.8179115466,1.3458027121\H,-1.4012669883,3.314
7918534,1.451433116\H,-1.5025266929,4.2616178727,-0.0402395033\H,-0.07
8230552,3.2551931565,0.2720795993\H,-3.7147802345,2.246490633,0.816162
0287\H,-3.9003584694,1.5070832327,-0.7908551087\H,-3.7021385884,3.2618
879768,-0.6339616529\c,0.7229378888,0.383410167,-0.9903035976\c,2.0986
976813,0.173658471,-1.0359923319\c,2.8658207599,0.1755547769,0.1314488
26\c,2.2266126024,0.3946438739,1.3532893216\c,0.8505613271,0.601088067
4,1.4012637791\H,0.133083468,0.3593047306,-1.9033624825\H,2.5825092848
,0.0016909699,-1.9949256794\c,4.3530745663,-0.0538054934,0.0699460717\
H,2.8052980464,0.3868174686,2.2732987129\H,0.3650203243,0.7672555746,2
.3613474951\c,4.8057057123,-1.3212920721,0.7664507569\H,4.9000811837,0
```

.7685148867,0.550910224\H,4.7100026057,-0.0898097149,-0.9638793193\O,4  
 .1668516212,-1.9821094429,1.544651009\O,6.0765414719,-1.6263108597,0.4  
 279747728\H,6.3243884046,-2.4259264281,0.924980752\Version=EM64L-G09R  
 evC.01\State=2-A\HF=-904.1722895\S2=0.754734\S2-1=0.\S2A=0.750014\RMSD  
 =2.030e-09\RMSF=3.704e-06\Dipole=0.6779545,0.1064228,0.6774567\Quadrupole=5.111596,-0.9611364,-4.1504596,-0.5005897,-5.4604758,0.8762706\PG=C01 [X(C16H24N1O3)]\\@

**19-P** (core)

1\1\GINC-R208\FOpt\RM062X\Gen\C14H19N1O3\ROOT\25-Aug-2014\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1073741824\psstnh\_core.freq\0,1\N,0.0054456372,-1.0819655124,0.4174095125\O,-1.2503467064,-1.4015611625,1.0048959105\C,-2.3047994608,-0.7974717892,0.2531600153\C,-3.553265558,-0.940550837,1.1107308363\C,-2.463326661,-1.4684233749,-1.0837642914\C,0.6412571586,-2.3478309327,0.0793714223\C,0.749001652,-0.3515466414,1.4452857622\C,2.0528917416,0.1740332621,0.8939337143\H,-3.4042970112,-0.4592993096,2.0813335887\H,-3.7760021805,-1.9990631636,1.2798359038\H,-2.0603768439,0.2639388575,0.1010615029\C,-2.2892374897,-0.8540738908,-2.2514017189\H,-1.9972768759,0.1931155301,-2.2953750639\H,0.9305789461,-0.986435249,2.3289308741\C,2.0631763502,0.9384646388,-0.2752828896\C,3.2605340391,1.432588719,-0.7849675306\C,4.4730028682,1.177157042,-0.1396373342\C,4.4627433594,0.4101577708,1.0264833792\C,3.2652687525,-0.0886119913,1.5337403937\H,1.1253615913,1.1305217891,-0.7905340854\H,3.2530436657,2.0248430461,-1.6973738875\C,5.7630270686,1.7231003261,-0.6935621554\H,5.3988328652,0.1852597989,1.5308529822\H,3.2739782819,-0.6939745961,2.4372148059\C,6.7387929836,0.655319283,-1.145052523\H,6.294933227,2.3192018947,0.0604796322\H,5.5831133919,2.3955583761,-1.5379163658\O,6.7042903514,-0.5158335454,-0.8671536696\O,7.7191151512,1.191981382,-1.903344292\H,8.3314260206,0.4716507207,-2.1356126157\H,0.0324442491,-2.8545380583,-0.6719720619\H,0.7496106172,-2.9969672933,0.962477309\H,1.627683102,-2.1375808959,-0.3421358196\H,0.1086140719,0.4797218198,1.7605795194\H,-4.4092127442,-0.4801671846,0.6093085898\H,-2.7406381193,-2.5235872594,-1.0473736976\H,-2.4252374883,-1.3692415697,-3.1977956521\Version=EM64L-G09RevC.01\State=1-A\HF=-824.9560689\RMSD=6.753e-09\RMSF=2.301e-06\Quadrupole=4.2412177,-3.555596,-0.6856217,2.795631,-0.5159326,-0.3341687\PG=C01 [X(C14H19N1O3)]\\@

**19-P**

1\1\GINC-R106\FOpt\RM062X\Gen\C32H41N1O3\ROOT\27-Aug-2014\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2415919104\psstnh.freq\0,1\N,0.506123365,-1.733208859,-0.582337834\O,1.7525628098,-1.1500063065,-0.9508807208\C,1.9790453467,0.0344772482,-0.1814235468\C,2.8811576112,0.9483003685,-1.0058530136\C,2.5067024277,-0.2631394866,1.2065272032\C,1.2466652542,-3.8645071159,-1.6971413925\C,-0.1799350089,-0.314523997,-2.6091953274\C,0.7279803491,-3.1957864288,-0.4151220052\C,-0.5775648345,-1.3792191362,-1.5561129288\C,1.7505943899,-3.4055642369,0.7043469341\C,-1.8167753583,-0.9590807213,-0.7782849796\C,-0.5979676107,-3.825874431,0.0256373974\H,-1.0161568468,-3.2847760558,0.8806750834\H,-0.4166753531,-4.8639114159,0.3225200616\H,1.8452467039,-4.4768457544,0.9123421936\H,1.4334190388,-2.8960242613,1.6200843243\H,2.7329527755,-3.0233608032,0.4197025865\H,1.4107298715,-4.9328316331,-1.5180135829\C,-1.414459233,0.2653281086,-3.3094485834\H,0.5398804145,-3.7735366244,-2.5290038429\C,0.7592787294,-0.9013624375,-3.6671847191\H,2.1979609201,-3.4174263495,-2.0012089414\H,0.3193098999,0.5130014065,-2.0927996023\H,2.4935570106,0.9712501686,-2.0332374689\C,2.9231086326,2.3807399717,-0.4396514627\H,3.8993070675,0.5447624854,-1.0634338687\H,1.0151137399,0.5334594323,-0.06546326\C,1.6689458783,-0.1134274726,2.3131716865\C,2.1198587441,-0.422190473,3.5969019644\C,3.4196302729,-0.8872262921,3.7841087007\C,4.2655965386,-1.0386895932,2.6840010118\C,3.8111301416,-0.7251736974,1.4059058758\H,0.6476716644,0.2303146679,2.1626580702\H,1.4535317501,-0.3077830308,4.4472352523\H,3.7734607812,-1.1331198038,4.7812275131\H,5.2787608093,-1.4049494573,2.8238718766\H,4.47039997,-0.8660784603,0.5521982271\H,3.3621277141,2.3333548826,0.5661580715\C,1.5153690697,2.9337942737,-0.2956316479\C,3.8107734747,3.277681404,-1.3080153567\C,0.9748001807,3.1932727043,0.9669469546\C,-0.3470538494,3.6188722886,1.1104510486\C,-1.1527695236,3.7879126368,-0.0134563176\C,-0.624380891,3.5387010833,-1.280478576\C,0.6974536704,3.1204719572,-1.4173592502\H,1.5932327424,3.0416111069,1.8494089481\H,-0.7460516058,3.8120430364,2.1027513463\H,-2.1853451033,4.1076371695,0.0938313426\H,-1.2449957771,3.6631916545,-2.1636494334\H,1.0907705335,2.91953089,-2.412654377\H,4.8290918204,2.8776225495,-1.3583396708\H,3.85801

64887, 4.2930211171, -0.9029071816\H, 3.4254317041, 3.3409601769, -2.331897  
 2786\H, -1.3470595212, -3.840165917, -0.7710402836\H, -0.8528460507, -2.269  
 7748773, -2.1411190569\H, -2.0183620333, -0.5298251416, -3.7659483789\H, -1  
 .0962993198, 0.9423559036, -4.110596587\H, -2.0581253292, 0.8244154547, -2.  
 6247120433\H, 0.2333096609, -1.6721342055, -4.2466547896\H, 1.6508541441, -  
 1.3478606868, -3.2252926618\H, 1.0740857962, -0.1212906222, -4.3707124131\br/>
 C, -1.7871860686, 0.1127330448, 0.1166644206\c, -2.9454588015, 0.5373447225  
 , 0.7614485308\c, -4.1667051788, -0.1016709553, 0.5371399856\c, -4.20208323  
 07, -1.1721720648, -0.3578221914\c, -3.0423095914, -1.5883427568, -1.006493  
 7138\H, -0.8584574366, 0.6455489164, 0.3025203739\H, -2.8944703356, 1.38265  
 15964, 1.4452740999\c, -5.4150833197, 0.3610363913, 1.2412985126\H, -5.1394  
 671998, -1.6918253228, -0.5393930801\H, -3.0927968509, -2.4212119193, -1.70  
 56319896\c, -5.9923248204, -0.658452572, 2.2021156737\H, -6.215277591, 0.58  
 24947675, 0.5217277007\H, -5.2411473856, 1.2883792167, 1.7956523449\o, -5.7  
 449284436, -1.8363137907, 2.2368215444\o, -6.8862819295, -0.081306882, 3.03  
 49994813\H, -7.2479275018, -0.7854417547, 3.601649017\Version=EM64L-G09R  
 evC.01\State=1-A\HF=-1523.8775546\RMSD=8.596e-09\RMSF=1.785e-06\Di pole  
 =-0.122735, 0.5882633, 0.1000336\Quadrupole=7.2056665, -9.2645252, 2.05885  
 87, -4.2652034, -1.0185779, 1.8026024\PG=C01 [X(C32H41N1O3)]\\@

**19-** (core)

1\1\GINC-R614\FOpt\UM062X\Gen\C10H11N1O3(1-,2)\ROOT\15-Aug-2014\0\#\#M0  
 62X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=80530  
 6368\stnc\_rcore.freq\,-1,2\N,2.3584116114,0.5186472609,-0.2674408612\br/>
 O,2.9413887726,0.4758173664,-1.4020550907\c,1.7925960167,1.7910276976,  
 0.1585413344\c,1.7795755124,-0.7178135694,0.2777053374\c,0.2791562912,  
 -0.7686217448,0.1120585913\H,2.0397613603,-0.7745878192,1.3424921948\c  
 , -0.29102245,-0.7841202793,-1.1629198697\c,-1.6762355953,-0.7742837325  
 ,-1.3120470367\c,-2.5351364368,-0.7507226883,-0.2037671287\c,-1.952572  
 1109,-0.7308693384,1.0723775062\c,-0.5686457732,-0.7355770774,1.222731  
 8917\H,0.3565147508,-0.7888670398,-2.0387642619\H,-2.1085006603,-0.777  
 9100774,-2.3104522442\c,-4.0247438771,-0.7200928489,-0.3745873022\H,-2  
 .610192332,-0.6611023292,1.9330654926\H,-0.1363361811,-0.7050204425,2.  
 2228256684\c,-4.7119004767,0.5815068137,0.2084965102\H,-4.4703637642,-  
 1.5594430679,0.1759272727\H,-4.2917433797,-0.8237735411,-1.4297838018\br/>
 O,-4.4108477259,0.8475393748,1.3937337743\o,-5.4959297222,1.1572874831  
 ,-0.5714425232\H,2.5157304336,2.5723785426,-0.0790140171\H,1.5919198326  
 6,1.7593741506,1.2341161435\H,0.8469087119,1.9823674231,-0.3624577509\br/>
 H,2.2895786978,-1.5237605167,-0.2555798292\Version=EM64L-G09RevC.01\State  
 =2-A\HF=-667.8512947\S2=0.755388\S2=1\o\S2A=0.750017\RMSD=3.586e-09\RMSF  
 =2.562e-06\Di pole=4.7938247,-1.6556228,0.2654474\Quadrupole=-37  
 .6587443,19.0697261,18.5890182,15.2337048,12.0763704,-0.4206927\PG=C01  
 [X(C10H11N1O3)]\\@

**19-**

1\1\GINC-R553\FOpt\UM062X\Gen\C16H23N1O3(1-,2)\ROOT\15-Aug-2014\0\#\#M0  
 62X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=13421  
 77280\stnc\_r.freq\,-1,2\N,-2.4385920768,-0.4206338922,-0.3868832501\o  
 ,-2.7207420671,-0.2870871391,-1.6241820903\c,-3.5406399436,-2.57719599  
 49,-0.3149416008\c,-2.4872323255,2.038983804,-0.1752360532\c,-2.276212  
 5882,-1.8207530846,0.1032652998\c,-1.8181903508,0.7378573488,0.2995610  
 52\c,-1.0397909968,-2.4528373629,-0.5507411642\c,-0.3117291553,0.72372  
 54317,0.1271540102\c,-2.1427658993,-1.8439589045,1.625376082\H,-1.2140  
 144988,-1.3737130816,1.9609929125\H,-2.1215484536,-2.8875058769,1.9559  
 272248\H,-1.003553878,-3.5211243032,-0.3084951172\H,-0.1151801258,-1.9  
 86113157,-0.1996075545\H,-1.0981885001,-2.3395736929,-1.6374729546\H,-  
 4.4294500363,-2.1133370749,0.1283027856\c,-1.868832615,3.2326200313,0.  
 5544357587\H,-3.6499497436,-2.5674951268,-1.401438539\c,-3.9988532016,  
 1.990446008,0.0543136803\H,-3.4769147429,-3.6147658564,0.0293731789\H,  
 -2.2943469356,2.1369512203,-1.2497358308\H,-2.9952658876,-1.3516944588  
 ,2.1085326299\H,-2.0452979461,0.628272236,1.3671148112\H,-2.005418349,  
 3.1379652525,1.6403719075\H,-2.3523660294,4.1633126627,0.2369805749\H,  
 -0.7962372933,3.3146839082,0.358058487\H,-4.218709648,1.838479783,1.12  
 03175886\H,-4.4619954785,1.1801275878,-0.5143877386\H,-4.4646386163,2.  
 9352128255,-0.2487608614\c,0.2659062273,0.6944034389,-1.1438425996\c,1.  
 6524562979,0.6607592149,-1.2829734766\c,2.5057897343,0.6577731887,-0.  
 1707057171\c,1.9155041085,0.6934141449,1.1018715271\c,0.5310118147,0.7  
 253166271,1.2426421785\H,-0.375468697,0.6671568011,-2.0231931568\H,2.0  
 894960823,0.6216889522,-2.2786642779\c,3.995160667,0.5890723816,-0.330  
 7859503\H,2.5659619912,0.645224621,1.9694415703\H,0.0931109798,0.74428  
 14919,2.2412806047\c,4.6500914997,-0.7106513456,0.292097131\H,4.457025  
 962,1.4329667382,0.1992086085\H,4.2712602906,0.6578131925,-1.386505768

7\O, 4.3201385346, -0.9498448055, 1.4753504163\O, 5.4429938898, -1.31185473  
 47, -0.4593473182\\Version=EM64L-G09RevC.01\\State=2-A\\HF=-903.6291259\\S  
 2=0.754789\\S2-1=0.\\S2A=0.750015\\RMSD=7.299e-09\\RMSF=1.937e-06\\Dipole=-  
 7.0887612, 1.6947197, 0.177681\\Quadrupole=-52.8938456, 26.2885291, 26.6053  
 165, 22.2554828, -10.4423417, 0.7162041\\PG=C01 [X(C16H23N1O3)]\\@

**19<sup>-</sup>P (core)**

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1\1\GINC-R3012\FOpt\RM062X\Gen\C14H18N1O3(1-)\\ROOT\27-Aug-2014\\#M06
2X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=107374
1824\\psstnc_core.freq\\-1,1\\N,0.2995369538,-1.411653378,-0.1331033509
\\O,1.5340282579,-1.4742030169,-0.8584028233\\C,2.3586007739,-0.38494548
12,-0.4804333623\\C,3.2850981411,-0.1086357627,-1.661473587\\C,3.1537636
561,-0.6628990398,0.7727615762\\C,-0.0134155325,-2.7780952026,0.2499113
543\\C,-0.6923331173,-0.8786336264,-1.0817127886\\C,-2.0365782508,-0.686
7243619,-0.4286169525\\H,2.7000327768,0.1670294191,-2.5436637181\\H,3.86
79037705,-1.0072261992,-1.8871268532\\H,1.7170261705,0.4902583066,-0.30
44987394\\C,3.3804474389,-1.8755595005,1.2716908664\\H,2.9580633135,-2.7
580207898,0.8000200597\\H,-0.774708149,-1.5473058829,-1.9557051235\\C,-3
.1529225179,-1.4069547852,-0.849393783\\C,-4.3915264943,-1.2251924269,-
0.2304618587\\C,-4.5527535901,-0.3239962004,0.8266903897\\C,-3.422579463
9,0.4021336372,1.2432758847\\C,-2.1907017077,0.2214148237,0.6269366763\\
H,-3.0557002162,-2.1167474947,-1.6702945986\\H,-5.2544297335,-1.7895788
31,-0.5778040301\\C,-5.8874316505,-0.1215506924,1.48163974\\H,-3.5531214
856,1.1378243792,2.0309151058\\H,-1.3247384999,0.7885978171,0.964969255
6\\C,-6.4613927324,1.343370127,1.3194948432\\H,-5.7878771267,-0.28456312
02,2.5630797757\\H,-6.6159705434,-0.8375912405,1.0913043598\\O,-5.695162
4079,2.2513915328,1.7126333765\\O,-7.6163893255,1.4108802494,0.85291628
69\\H,3.9795826744,0.7039006794,-1.4248564655\\H,3.5877141091,0.21454583
14,1.2538098158\\H,-0.9906315738,-2.772505438,0.7379103901\\H,0.73921379
45,-3.1332275318,0.9561100853\\H,-0.0474377867,-3.4497124092,-0.6241191
554\\H,-0.2949652901,0.0810782107,-1.4343466199\\H,3.9848653647,-2.01811
26016,2.1625239677\\Version=EM64L-G09RevC.01\\State=1-A\\HF=-824.4084378
\\RMSD=9.151e-09\\RMSF=2.438e-06\\Dipole=7.764829,-3.4972081,-1.3581118\\Q
uadrupole=-50.862975,17.8489334,33.0140416,41.7919006,14.6490452,-8.49
15544\\PG=C01 [X(C14H18N1O3)]\\@

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**19<sup>-</sup>P**

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1\1\GINC-R3011\FOpt\RM062X\Gen\C32H40N1O3(1-)\\ROOT\28-Aug-2014\\#M06
2X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=241591
9104\\psstnc.freq\\-1,1\\N,-0.088768114,-1.8179066857,0.7318748976\\O,-1
.511067825,-1.7660877413,0.8597924147\\C,-2.0377628842,-0.8168443407,-0
.0743696252\\C,-3.3162010276,-0.2225065601,0.513380701\\C,-2.2283681266,
-1.4185720354,-1.4519759694\\C,-0.0999689568,-3.9874091263,2.006189683\\
C,-0.356599279,-0.1087443811,2.6189563635\\C,0.3129775065,-3.2457613927
,0.7242934974\\C,0.6029397955,-0.9858280421,1.7733574253\\C,-0.34417076,
-3.9309778567,-0.4769615858\\C,1.6807876884,-0.1410921711,1.1142930082\\
C,1.8335317484,-3.3008100018,0.5316153957\\H,2.1277160315,-2.706177112,
-0.3390244782\\H,2.1342747762,-4.3419934705,0.3701343358\\H,0.0343746441
,-4.9559875863,-0.56429221\\H,-0.1152771852,-3.3901226266,-1.4010877236
\\H,-1.4296661357,-3.97233923,-0.3635290583\\H,0.2010190228,-5.039699441
3,1.9423971255\\C,0.396178079,0.9892355621,3.3770495553\\H,0.3679702883,
-3.5598813344,2.8992271955\\C,-1.150485412,-0.9521508687,3.6218090567\\H
,-1.1864739055,-3.946315323,2.1327176668\\H,-1.044822269,0.396587533,1.
9346284455\\H,-3.1293791395,0.0068122673,1.5707623622\\C,-3.741707697,1.
067019732,-0.221099593\\H,-4.1368764353,-0.9511870207,0.4868389201\\H,-1
.3104841096,-0.0092468793,-0.1606892778\\C,-1.4004525653,-1.028466903,-
2.5062227297\\C,-1.5380807746,-1.6022610283,-3.7708765011\\C,-2.50763933
9,-2.5778128163,-3.9922488121\\C,-3.3408711453,-2.9743279425,-2.9443264
434\\C,-3.2020159483,-2.3947147463,-1.6861016322\\H,-0.6326898218,-0.278
7545059,-2.3291412894\\H,-0.8816572462,-1.2909623988,-4.5787715107\\H,-2
.6142680301,-3.0295705158,-4.9748028517\\H,-4.0959775994,-3.7385161963,
-3.109097965\\H,-3.8398495872,-2.7227760131,-0.8678835888\\H,-3.97071571
42,0.7996924201,-1.2626096641\\C,-2.5986931706,2.069901672,-0.250479249
7\\C,-5.011260958,1.6442595217,0.4124324404\\C,-1.9591902969,2.389037825
3,-1.4524846591\\C,-0.8205768675,3.1979355712,-1.4703598858\\C,-0.291212
6477,3.7090657656,-0.2853148085\\C,-0.9464584169,3.4234175861,0.9140727
989\\C,-2.0849506175,2.617624402,0.9314719221\\H,-2.3417515894,1.9688577
355,-2.3820010372\\H,-0.3210735535,3.4097972068,-2.4125969579\\H,0.64380
02538,4.271196434,-0.2940315057\\H,-0.5460452158,3.8106681158,1.8473730
026\\H,-2.5576616131,2.3844371285,1.8857315879\\H,-5.8275164018,0.912890
9488,0.3842396822\\H,-5.334701459,2.5468573968,-0.1154363027\\H,-4.83786
73993,1.9131249914,1.4606931078\\H,2.3853286793,-2.9233516274,1.3969637

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23\H,1.100707981,-1.6460560096,2.5014247716\H,1.1651697307,0.561737226
6,4.0339318007\H,-0.3106846955,1.5451854196,4.0054026922\H,0.887550018
4,1.6954136097,2.7031387636\H,-0.4664184106,-1.393727568,4.3601743327\
H,-1.7054582943,-1.75753298,3.1376872975\H,-1.8619198758,-0.3225807891
,4.1710681783\C,2.9383166723,-0.0110055927,1.7036312781\C,3.8633289698
,0.922181845,1.2289824541\C,3.5663275919,1.7522778997,0.1427645811\C,2
.3221693774,1.5776179506,-0.4799351034\C,1.4015699418,0.654620927,-0.0
01182987\H,3.1885028604,-0.6215281968,2.5720687272\H,4.8253840335,1.02
67273569,1.7267909457\C,4.5009412417,2.8340676947,-0.3129256588\H,2.06
70112838,2.2249042232,-1.3132466873\H,0.4345778316,0.5809669948,-0.488
9329429\C,3.9227450161,4.2863250008,-0.0818395962\H,4.6702783304,2.745
4958329,-1.3943562617\H,5.4668126569,2.7530656561,0.1930499129\O,2.765
0250794,4.4746755471,-0.5334159253\O,4.6896643859,5.0823230572,0.49004
60286\Version=EM64L-G09RevC.01\State=1-A\HF=-1523.339704\RMSD=9.079e-
09\RMSF=7.693e-06\Dipole=-5.4958759,-6.5620662,-0.1485194\Quadrupole=-
10.4411591,-31.5398685,41.9810276,-50.6368456,-2.1325581,0.9457792\PG=
C01 [X(C32H40N1O3)]\@\@
```

**20** (core)

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1\1\GINC-R3457\FOpt\UM062X\Gen\C9H10N1O3(2)\ROOT\01-Sep-2014\0\#M062X
/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=13421772
80\mtnh_rcore.freq\0,2\N,2.1151809613,-0.159717546,0.1559658259\O,2.
7074238703,0.0039049756,1.2731362604\C,2.0105854273,-1.5173412132,-0.3
621526631\C,1.0808861533,0.8095210041,-0.2100184271\C,-0.265168468,0.4
407341731,0.3783284161\H,1.0186354492,0.856886231,-1.3020352567\C,-1.3
573291944,0.179311582,-0.4423331468\C,-2.5886052347,-0.1792045093,0.11
46662508\C,-2.7321604311,-0.2857557762,1.4981026722\C,-1.6355801214,-0
.0323716175,2.3214393886\C,-0.4109657821,0.3290989662,1.76732694\H,-1.
2762050047,0.2505162064,-1.524394671\C,-3.7190644896,-0.4436836881,-0.
8157892542\H,-1.738102409,-0.1154757387,3.3990212136\H,0.4487079742,0.
5191039438,2.4059018068\O,-3.6488997095,-0.37846231,-2.0209928372\O,-4
.8612046448,-0.7724974427,-0.1787720082\H,-5.5350337978,-0.9236187189,
-0.8638610618\H,-3.6912179747,-0.5652507221,1.9209094677\H,1.765904440
4,-1.483611127,-1.4267088562\H,1.2288426634,-2.0708143525,0.1734710896
\H,2.9734651724,-2.0051284346,-0.2095113502\H,1.43203515,1.7723561146,
0.1690402006\Version=ES64L-G09RevD.01\State=2-A\HF=-629.1040923\S2=0.
755151\S2-1=0.\$2A=0.750015\RMSD=5.034e-09\RMSF=6.719e-06\Dipole=-0.69
47156,-0.2917252,-0.1310516\Quadrupole=-1.2154909,1.9123744,-0.6968835
,-0.0233839,-8.0999914,0.2816996\PG=C01 [X(C9H10N1O3)]\@\@
```

**20**

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1\1\GINC-R100\FOpt\UM062X\Gen\C15H22N1O3(2)\ROOT\14-Aug-2014\0\#M062X
/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=10737418
24\mtnh_r.freq\0,2\N,-2.1483280826,-0.3375211337,-0.3648417234\O,-2.
2520723286,-0.2896286014,-1.6345679815\C,-3.7410268105,-2.1597256658,-
0.2216846985\C,-1.7629431844,2.1029521909,-0.3238762\C,-2.3767056763,-
1.6690948946,0.2695541377\C,-1.3732882526,0.7416043795,0.2805820603\C,
-1.2699525818,-2.6309535812,-0.1829094238\C,0.1144436439,0.4492968532,
0.1902548297\C,-2.388072095,-1.5453809776,1.7921252214\H,-1.4073199756
,-1.2698256551,2.1931219527\H,-2.6542296226,-2.5177785888,2.2176879261
\H,-1.4857139381,-3.6405037139,0.1831227916\H,-0.2931565302,-2.3246031
811,0.2053393967\H,-1.2226850074,-2.6555012491,-1.2756063268\H,-4.5304
639346,-1.4645807132,0.0841965578\C,-0.9891547138,3.2233163036,0.37356
51983\H,-3.7506293533,-2.238312079,-1.3106057025\C,-3.2707102434,2.327
2224512,-0.2028622841\H,-3.9543462011,-3.1430314814,0.2091607687\H,-1.
4923458421,2.0847819745,-1.3860806714\H,-3.1328468243,-0.8156079847,2.
1293001103\H,-1.6599749698,0.7585149937,1.3370702647\H,-1.2010108824,3
.2330522667,1.4508640064\H,-1.2870470233,4.1954913981,-0.0316466983\H,
0.09231646,3.1201177756,0.2435444103\H,-3.5810440053,2.2930905133,0.85
01662488\H,-3.8328841125,1.5704878951,-0.7556810204\H,-3.5422971356,3.
3119785546,-0.5967789879\C,0.8966585455,0.410737598,1.3404477812\C,2.2
656883663,0.1402267068,1.2586526086\C,2.8644336398,-0.0961012367,0.020
6837696\C,2.0829524689,-0.056165854,-1.1332505753\C,0.7198574775,0.215
4638412,-1.0514544099\H,0.4595333054,0.5915578023,2.3202335485\C,3.043
0829957,0.1094639839,2.5265312753\H,2.5393196394,-0.2409571042,-2.1009
704153\H,0.1068890795,0.2284973823,-1.9494906381\O,2.5763036081,0.2941
495905,3.626597319\O,4.353005554,-0.1509086916,2.3371766256\H,4.771704
7851,-0.1488361649,3.2151333836\H,3.9267557578,-0.3086449035,-0.033831
436\Version=EM64L-G09RevC.01\State=2-A\HF=-864.8830057\S2=0.754748\S2-
1=0.\$2A=0.750014\RMSD=4.178e-09\RMSF=1.999e-06\Dipole=0.3359052,-0.2
536047,0.2191679\Quadrupole=5.787611,1.0365534,-6.8241644,-0.517438,-4
.4357453,-1.9281645\PG=C01 [X(C15H22N1O3)]\@\@
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**20-P** (core)

```
1\1\GINC-R122\FOpt\RM062X\Gen\C13H17N1O3\ROOT\16-Aug-2014\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1073741824\psmtnh_core.freq\0,1\N,-0.3452786278,-0.6061746112,0.5261214228\0,0.7155045852,-1.4469336366,0.087363998\c,1.9425772805,-0.7125427247,0.0615131102\c,1.9223131909,0.3474716742,-1.0352527178\c,3.0214132596,-1.7304793351,-0.1726350624\c,-0.7807284339,-1.1453457398,1.8098596288\c,-1.3896176747,-0.7213890505,-0.4938571435\c,-2.5400359677,0.2095837325,-0.1935564026\h,1.0932306226,1.0421330909,-0.8720561331\h,1.8028968727,-0.1266451492,-2.0158650637\h,2.0874004699,-0.2356862768,1.0416515591\c,4.1026339637,-1.8569833361,0.5926810243\h,4.2497465481,-1.2342609023,1.4726028224\h,-1.7471135589,-1.7609722897,-0.5752777709\c,-2.3036101882,1.5757174967,0.0062401452\c,-3.3535398707,2.4491287542,0.2743137196\c,-4.6612376513,1.971333067,0.3469714456\c,-4.9025082844,0.6111574204,0.1522827999\c,-3.8452936821,-0.2649604683,-0.1124798413\h,-1.2820017322,1.944544888,-0.0401507272\h,-3.1548182079,3.5056284754,0.4267190607\c,-6.274609893,0.0408805859,0.2238090038\h,-4.0645357008,-1.320501382,-0.2521311537\h,-5.4878730316,2.6424673086,0.5540403228\o,-6.5461307763,-1.1269115647,0.0690029148\o,-7.2194707407,0.9683845655,0.4849524933\h,-8.0726250917,0.5020171262,0.5111512437\h,-1.5993659302,-0.5281768536,2.1888600289\h,0.0552589684,-1.0963916676,2.5107850278\h,-1.1158919395,-2.1897374941,1.719017101\h,-0.9253134014,-0.4545717315,-1.4491378107\h,2.8594951647,0.9121360515,-1.0337723574\h,2.8826759757,-2.3650421848,-1.0482585284\h,4.8784834828,-2.5824978383,0.3682218401\Version=EM64L-G09RevC.01\State=1-A\HF=-785.665667\RMSD=8.530e-09\RMSF=6.961e-06\Di pole=0.3275315,0.8862794,0.1925444\Quadrupole=4.5840194,-2.7552045,-1.8288149,-4.4293785,-1.2092596,0.6447526\PG=C01 [X(C13H17N1O3)]\\@
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**20-P**

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1\1\GINC-R2034\FOpt\RM062X\Gen\C31H39N1O3\ROOT\17-Aug-2014\0\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2147483648\psmtnh.freq\0,1\N,0.301679729,-1.4951177,-0.8671587271\o,1.2290126134,-0.5335481002,-1.3394391529\c,1.7776235105,0.2503531694,-0.2664435287\c,0.9983954483,1.5597674137,-0.1073899617\c,3.2316563339,0.497893665,-0.602127214\c,1.261301039,-3.1385717758,-2.5113688669\c,-1.2037831131,-0.0680894103,-2.3591243791\c,0.912032594,-2.843551828,-1.046530602\c,-1.0420490264,-1.3408116815,-1.4889660716\c,2.1910642171,-2.9004403777,-0.2056533164\c,-2.0820987585,-1.444609978,-0.3801170017\c,-0.0664178718,-3.8885174683,-0.4975323591\h,-0.3598199529,-3.6415561005,0.5281186748\h,0.4260095532,-4.8662796734,-0.4925130111\h,2.619741784,-3.9067423784,-0.2581282362\h,1.9723209059,-2.6748187027,0.8442865708\h,2.9417972886,-2.1954668975,-0.5732522692\h,1.7269461986,-4.1268381943,-2.591603206\c,-2.6741519476,0.2478104713,-2.6503634996\h,0.375207394,-3.1365162712,-3.155236509\c,-0.4552441446,-0.2275797485,-3.6865422075\h,1.9679012086,-2.3935304516,-2.8895973494\h,-0.7788053703,0.7773608222,-1.8120369481\h,-0.0540531105,1.3226476597,0.0971608386\c,1.5302769853,2.484117154,0.9996022931\h,1.0230001888,2.0960969327,-1.0662004106\h,1.7080681001,-0.3352647437,0.6575335024\c,4.2398532045,0.1846942389,0.3108189683\c,5.5774944479,0.4397386695,0.0070388405\c,5.9180659156,1.00144597,-1.2216086927\c,4.9168162556,1.3029937453,-2.1459776513\c,3.5818909182,1.0549916169,-1.8362726329\h,3.9731164009,-0.2667779137,1.2643904915\h,6.3524682473,0.1912702641,0.7266866468\h,6.9588680508,1.1977094747,-1.4621423513\h,5.1779108344,1.7310876193,-3.1096279261\h,2.8025171594,1.2811737047,-2.5607004531\h,2.5827527273,2.7066469827,0.7791103937\c,1.4796419591,1.8164451906,2.36182796\c,0.7557761787,3.8081227634,1.0012925927\c,2.6469867946,1.607189448,3.1005025829\c,2.6079888823,0.9833877077,4.3481150494\c,1.3922388082,0.5600102734,4.8793659739\c,0.216974751,0.7746878572,4.1587643778\c,0.2619797762,1.3990396347,2.9144924322\h,3.599172217,1.9353550889,2.6886243267\h,3.5287362985,0.8302690934,4.9041860459\h,1.3575317283,0.0725227825,5.8491363911\h,-0.7372901218,0.4595995027,4.5722633857\h,-0.6653222163,1.569496661,2.369538206\h,0.8542711788,4.3132617061,0.0345431528\h,1.1295090671,4.4780009508,1.7816800741\h,-0.3112250164,3.6389599551,1.1855862322\h,-0.9745714438,-3.9821897498,-1.1003640876\h,-1.2309519332,-2.1762597809,-2.1800890017\h,-3.1734521851,-0.5953325092,-3.1443061928\h,-2.7331857091,1.1064865605,-3.327562832\h,-3.2392055732,0.4895994286,-1.7461083442\h,-0.9112365177,-1.0303943132,-4.2812440454\h,0.599649025,-0.4635094799,-3.5370421029\h,-0.5238809072,0.695370445,-4.2733811006\c,-1.8509067031,-0.9024495567,0.8875566216\c,-2.828118034,-0.9543455433,1.8803639907\c,-0.0516684005,-1.5699549411,1.6321117167\c,-4.2788651155,-2.1420333419,0.3779617088\c,-3.2995119076,-2.0809324093,-0.6152945132\h,-0.877947938
```

5,-0.4711647358,1.1034550988\H,-2.6260442103,-0.5257381633,2.858167540  
 1\C,-5.5511630332,-2.8404216519,0.0545462289\H,-3.5081011502,-2.546016  
 8148,-1.5764299252\H,-4.8169313037,-1.6237589715,2.3989034295\O,-5.803  
 4361074,-3.3651977664,-1.0054697629\O,-6.4311990971,-2.8388508166,1.07  
 84332224\H,-7.2216199985,-3.3141986831,0.7699438813\\Version=EM64L-G09  
 RevC.01\\State=1-A\\HF=-1484.5859025\\RMSD=9.495e-09\\RMSF=1.469e-06\\Dipol  
 e=0.6623833,0.4118902,0.5984564\\Quadrupole=4.275021,-4.9769228,0.70190  
 18,-0.5143174,-5.5352969,-6.0395322\\PG=C01 [X(C31H39N1O3)]\\@

**20<sup>-</sup>** (core)

1\\1\\GINC-R3459\\FOpt\\UM062X\\Gen\\C9H9N1O3(1-,2)\\ROOT\\01-Sep-2014\\0\\#M06  
 2X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=134217  
 7280\\mtnc\_rcore.freq\\-1,2\\N,2.0862824143,-0.2013590329,0.0700646417\\  
 0,2.9119692333,-0.0617477264,1.0334066108\\C,1.7575669577,-1.5566538243  
 ,-0.3485045002\\C,1.0921384706,0.8552829856,-0.1698902712\\C,-0.25803597  
 07,0.506047255,0.4143051997\\H,1.0029974962,0.9968041105,-1.2534980665\\  
 C,-1.3253050565,0.1732296675,-0.4202895687\\C,-2.5638586915,-0.20717101  
 93,0.1016744121\\C,-2.7196060897,-0.2517342522,1.4871652897\\C,-1.657505  
 3164,0.0747253535,2.3341962955\\C,-0.4253345681,0.452097854,1.802943499  
 8\\H,-1.2292745898,0.1972723209,-1.5047176835\\C,-3.7329843504,-0.581791  
 0492,-0.8480085226\\H,-1.7882216684,0.0351689662,3.4137191902\\H,0.41191  
 91174,0.6956241026,2.4552145044\\O,-3.4601627432,-0.5228048729,-2.06805  
 50857\\O,-4.7987169404,-0.898302284,-0.2763965306\\H,-3.6906529813,-0.54  
 99547194,1.8727996501\\H,1.2682171438,-1.5263245774,-1.3253325033\\H,1.0  
 730527995,-2.0200255054,0.372320745\\H,2.6876405862,-2.124760946,-0.399  
 6032965\\H,1.5227647473,1.7548171935,0.2764059902\\Version=ES64L-G09Rev  
 D.01\\State=2-A\\HF=-628.5646144\\S2=0.755382\\S2-1=0.\\S2A=0.750017\\RMSD=4  
 .205e-09\\RMSF=8.121e-06\\Dipole=3.9512316,0.5362451,1.3989341\\Quadrupol  
 e=-30.4245852,19.9829697,10.4416154,-7.500434,-19.5348248,-2.163388\\PG  
 =C01 [X(C9H9N1O3)]\\@

**20<sup>-</sup>**

1\\1\\GINC-R111\\FOpt\\UM062X\\Gen\\C15H21N1O3(1-,2)\\ROOT\\15-Aug-2014\\0\\#M0  
 62X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=10737  
 41824\\mtnc\_r.freq\\-1,2\\N,2.1611689775,-0.107828425,0.158165401\\O,2.7  
 458465473,0.1219544096,1.2691885156\\C,3.7153928076,-1.8953928313,-0.35  
 31229626\\C,1.5012806987,2.2713397455,0.0677871034\\C,2.2328916302,-1.51  
 05202792,-0.3445224123\\C,1.0872699257,0.826652325,-0.2564987153\\C,1.45  
 29368199,-2.4307234665,0.6050488227\\C,-0.2432544687,0.4174525791,0.349  
 2812391\\C,1.6670831385,-1.6056457528,-1.7609195198\\H,0.5916929222,-1.4  
 086348536,-1.7909573752\\H,1.8261615862,-2.6243287104,-2.1298625085\\H,1  
 .6169495617,-3.4759915938,0.3180231093\\H,0.3797890715,-2.2224933438,0.  
 5685878458\\H,1.8044300233,-2.285521595,1.6312217749\\H,4.2806369369,-1.  
 2251768605,-1.0109343298\\C,0.4051039321,3.2348362236,-0.3907568601\\H,4  
 .1344534211,-1.8278828556,0.6531841882\\C,2.8363736332,2.6171506291,-0.  
 5942367207\\H,3.8252757885,-2.9215218726,-0.7198141205\\H,1.6153891269,2  
 .3487195293,1.155354171\\H,2.1799811588,-0.9157152021,-2.4413605095\\H,  
 1.005523972,0.7475942585,-1.3466123167\\H,0.233181641,3.1436315675,-1.4  
 713186713\\H,0.6996409719,4.2699020091,-0.1833725963\\H,-0.5447228637,3.  
 0366164279,0.1132757824\\H,2.7642139859,2.4978392524,-1.6841411778\\H,3.  
 6413999597,1.9751379819,-0.2270816273\\H,3.1069074631,3.6600208069,-0.3  
 921822372\\C,-1.3271811302,0.1233849363,-0.4785835648\\C,-2.5564550073,-  
 0.2817101584,0.0464489049\\C,-2.6898970314,-0.3830910021,1.4315077769\\C  
 ,-1.6145995454,-0.0842455819,2.2719121056\\C,-0.3901762495,0.3146602016  
 ,1.7373220361\\H,-1.251512705,0.1956649062,-1.5629999753\\C,-3.737354903  
 2,-0.624074272,-0.900765548\\H,-1.7259665959,-0.1694732366,3.3510570285  
 \\H,0.4595340117,0.5203225942,2.3858078435\\O,-3.480042191,-0.5220911881  
 ,-2.1214773243\\O,-4.7953016806,-0.9621328977,-0.3272879949\\H,-3.652585  
 3409,-0.7025844045,1.8210454186\\Version=EM64L-G09RevC.01\\State=2-A\\HF  
 =-864.3425816\\S2=0.754809\\S2-1=0.\\S2A=0.750015\\RMSD=9.940e-09\\RMSF=1.9  
 64e-06\\Dipole=5.9410924,0.7876933,1.0876018\\Quadrupole=-41.0968128,24.  
 275372,16.8214407,-11.9898817,-19.7103154,-2.2193644\\PG=C01 [X(C15H21N  
 1O3)]\\@

**20<sup>-P</sup>** (core)

1\\1\\GINC-R122\\FOpt\\RM062X\\Gen\\C13H16N1O3(1-)\\ROOT\\20-Aug-2014\\0\\#M062  
 X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1073741  
 824\\psmtnc\_core.freq\\-1,1\\N,0.4838166645,-1.0307477429,-0.3705638078  
 \\O,-0.6787338767,-1.6842953691,0.1407668164\\C,-1.7300021793,-0.7389122  
 137,0.2552713377\\C,-1.4447080881,0.2847907821,1.352648994\\C,-3.0056869  
 283,-1.4871776567,0.5234913825\\C,0.7302134905,-1.6097750213,-1.6822970  
 635\\C,1.5651416705,-1.3279034868,0.5763218555\\C,2.8535134363,-0.662852  
 6181,0.1570839185\\H,-0.5236787489,0.8269918939,1.1238033097\\H,-1.33898

06949, -0.2247654853, 2.3163953241\H, -1.8245628063, -0.207804311, -0.70600  
 32217\C, -3.11651212, -2.8093329708, 0.6410829259\H, -2.249857173, -3.45337  
 99498, 0.5322617356\H, 1.7007109298, -2.4207009423, 0.6626937458\C, 3.95226  
 60687, -1.4262757225, -0.2443369629\C, 5.1326700616, -0.7959852439, -0.6454  
 156994\C, 5.2140095885, 0.5952043174, -0.6500474068\C, 4.122814284, 1.37379  
 92648, -0.2521545633\C, 2.9516263551, 0.7323025129, 0.1488131588\H, 3.88222  
 07909, -2.5135271024, -0.2436477886\H, 5.9859879543, -1.3964193216, -0.9546  
 980387\C, 4.2150907742, 2.9235347162, -0.2510663161\H, 2.1136417333, 1.3572  
 756756, 0.4505750296\H, 6.1157711993, 1.1179917852, -0.9566922432\O, 3.1856  
 75025, 3.5154549243, 0.1421153735\O, 5.3086158125, 3.3878398321, -0.6433328  
 889\H, -0.1387594474, -1.4202354893, -2.3177380115\H, 0.9072668165, -2.6969  
 126269, -1.6237528824\H, 1.6057526996, -1.119247537, -2.1131943488\H, 1.232  
 6856742, -0.9531888262, 1.5500459846\H, -3.8849215758, -0.8528450763, 0.640  
 8445146\H, -4.0757318169, -3.2748198832, 0.8496243788\H, -2.2634355741, 1.0  
 089788929, 1.4263014576\\Version=EM64L-G09RevC.01\\State=1-A\\HF=-785.122  
 1269\\RMSD=4.707e-09\\RMSF=2.524e-06\\Dipole=-4.1529704, -5.2610083, 0.1837  
 201\\Quadrupole=-3.5467991, -20.0343226, 23.5811217, -33.765731, 3.0280365,  
 3.2198388\\PG=C01 [X(C13H16N1O3)]\\@

20^-P

1\\1\\GINC-R3084\\FOpt\\RM062X\\Gen\\C31H38N1O3(1-)\\ROOT\\23-Aug-2014\\0\\#M06  
 2X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=214748  
 3648\\psmtnc.freq\\-1,1\\N,-0.4807860302,-1.2232900293,0.4921019403\\O,0  
 .7244232493,-1.5530382097,-0.1833705202\C,1.696092796,-0.4981577535,-0  
 .0990154766\C,1.6168089353,0.4124689681,-1.3273969764\C,3.0459451424,-  
 1.1733751214,0.0142612247\C,-0.4476983431,-3.5713365751,1.3905810039\C  
 ,-1.3264986714,-1.4618512429,-1.8994251724\C,-0.5396956597,-2.07215844  
 82,1.7154482537\C,-1.6753356659,-1.3514213428,-0.3941396229\C,0.635550  
 942,-1.6873752813,2.6209876031\C,-2.6279286892,-0.2041347525,-0.087628  
 5966\C,-1.8379918395,-1.760518697,2.4683902231\H,-1.9434882025,-0.6830  
 241944,2.6280682539\H,-1.807686964,-2.2624210035,3.4420516944\H,0.5684  
 582336,-2.2426569831,3.563438328\H,0.6077899324,-0.6160914011,2.847929  
 8061\H,1.5957612969,-1.9306775588,2.1565921337\H,-0.4771924775,-4.1556  
 725735,2.317640194\C,-2.5310589482,-1.1407569748,-2.7895323378\H,-1.27  
 85770573,-3.905523666,0.7595127272\C,-0.8195826363,-2.868159351,-2.240  
 3047836\H,0.4916298382,-3.789295453,0.8725958731\H,-0.5426503682,-0.73  
 30394348,-2.1210493642\H,0.6316102015,0.8960649344,-1.3345700284\C,2.7  
 147357036,1.4856392178,-1.4030352317\H,1.6759688004,-0.2185266591,-2.2  
 263286266\H,1.4962535279,0.0914251049,0.8015882213\C,3.9670554844,-0.7  
 808451654,0.9868793312\C,5.222061843,-1.386277656,1.060953139\C,5.5635  
 904251,-2.4001976928,0.1679059627\C,4.64276828,-2.8071563987,-0.798987  
 7524\C,3.3935840633,-2.1957314601,-0.8753733773\H,3.6992823876,0.01065  
 79033,1.6834552977\H,5.9300843731,-1.0671050663,1.8212013657\H,6.53962  
 6705,-2.8744739848,0.2263043905\H,4.899287333,-3.6026359702,-1.4937819  
 566\H,2.6710055262,-2.51577114,-1.6228392823\H,3.6844578348,0.97389855  
 42,-1.4848293154\C,2.7611623205,2.369754598,-0.1695991961\C,2.51634098  
 2,2.3386947167,-2.6634786756\C,3.9671702702,2.5935910801,0.5031490637\  
 C,4.0153964601,3.4212336008,1.6255793903\C,2.851862904,4.0374031422,2.  
 0886740251\C,1.6447712234,3.827724411,1.4206041587\C,1.6044742078,3.00  
 19147659,0.2982039294\H,4.8735593105,2.10321765,0.1495060829\H,4.96131  
 79044,3.5816670884,2.1381044455\H,2.8881936715,4.6798336883,2.96504240  
 37\H,0.7121101101,4.2881937634,1.7360415058\H,0.6351128055,2.881787098  
 9,-0.1826086257\H,2.513065693,1.7121359656,-3.5636248217\H,3.315440662  
 ,3.0813119178,-2.7584188812\H,1.5626827594,2.8756909362,-2.613917858\H  
 ,-2.7284598595,-2.1109318103,1.9391511525\H,-2.2129255211,-2.286624155  
 8,-0.1626619801\H,-3.3780999481,-1.8003514072,-2.5599129978\H,-2.26040  
 70993,-1.2982266411,-3.8403792619\H,-2.8713413179,-0.1095307959,-2.668  
 1266018\H,-1.6330465554,-3.5967738917,-2.1158168419\H,0.0136175956,-3.  
 1701802142,-1.6028474553\H,-0.4927438344,-2.9157292243,-3.2864583881\C  
 ,-4.0026153631,-0.4466660702,-0.0215404301\C,-4.8958347756,0.601653102  
 9,0.2009593821\C,-4.4192809416,1.90158581,0.3638274019\C,-3.0478748233  
 ,2.1614987002,0.3141137664\C,-2.1660592791,1.1011810029,0.0933324647\H  
 ,-4.3755667451,-1.4644645305,-0.1406057916\H,-5.9634502307,0.398238893  
 9,0.2551674734\C,-2.5205259751,3.6022632715,0.5205260089\H,-1.10056729  
 84,1.3145138426,0.097727072\H,-5.0848521444,2.7407677071,0.5447729173\  
 O,-1.2712460162,3.7265459898,0.4642314398\O,-3.3917354536,4.4713765556  
 ,0.7219801774\\Version=EM64L-G09RevC.01\\State=1-A\\HF=-1484.0511867\\RMS  
 D=3.353e-09\\RMSF=2.289e-06\\Dipole=3.7549244,-5.5156804,-0.6173685\\Quad  
 rupole=-3.2508625,-24.9232355,28.174098,29.0142761,3.9966389,-4.106737  
 8\\PG=C01 [X(C31H38N1O3)]\\@

**21 (core)**

```
1\1\GINC-R3458\FOpt\UM062X\Gen\C10H12N1O3(2)\ROOT\01-Sep-2014\0\\#M062
X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177
280\\smtnh_rcore.freq\\0,2\N,2.3845428847,0.1327527818,0.0466670514\O,
3.0498975327,0.2240618617,1.1305299866\C,2.520176133,-1.092929599,-0.7
284507091\C,1.1308339128,0.8829203179,-0.0481211263\C,-0.0391868495,0.
0959836877,0.505280256\H,0.9562035767,1.1371386989,-1.0989216694\C,-1.
1293455323,-0.2221836394,-0.3010122171\C,-2.204130316,-0.9631828477,0.
2031983782\C,-2.1739851088,-1.3863467641,1.5300727861\C,-1.078794547,-
1.0811535248,2.3409612127\C,-0.0148235648,-0.3433407722,1.8343699\H,-1
.1561610984,0.1162729758,-1.3362624493\C,-4.1517687342,0.0003125156,-0
.9755153973\H,-1.0607928686,-1.4195873652,3.3727153902\H,0.8452691829,
-0.1089146717,2.4570615635\O,-3.9561913137,0.7318912827,-1.9149828493\
O,-5.0645990929,0.265367666,-0.021819788\H,-5.4746591344,1.1213464055,
-0.2390148231\H,-3.0079724126,-1.9557853078,1.9324500931\C,-3.38892629
6,-1.2735828155,-0.6919065978\H,-4.0499934212,-1.9981894918,-0.2106439
856\H,-3.0521622556,-1.6718145862,-1.6523199493\H,2.1577287885,-0.9227
267611,-1.7454451277\H,1.9403333806,-1.9020672887,-0.2664394041\H,3.57
67117271,-1.3612647862,-0.7422909492\H,1.2963554271,1.8029220279,0.517
6404248\\Version=ES64L-G09RevD.01\\State=2-A\\HF=-668.3937519\\S2=0.75515
3\\S2-1=0.\\S2A=0.750016\\RMSD=3.161e-09\\RMSF=8.862e-07\\Dipole=-0.935637,
-0.5876447,-0.3132863\\Quadrupole=-3.5668635,3.6670045,-0.1001409,-1.73
83288,-8.9969096,1.1327115\\PG=C01 [X(C10H12N1O3)]\\@
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**21**

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1\1\GINC-R393\FOpt\UM062X\Gen\C16H24N1O3(2)\ROOT\15-Aug-2014\0\\#M062X
/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=13421772
80\\smtnh_r.freq\\0,2\N,2.0169491018,-0.146865179,0.180576321\O,2.5165
033493,0.001741674,1.3440395059\C,3.6166826628,-1.8841536517,-0.368501
2402\C,1.4368394798,2.2552213659,0.1503036787\C,2.1337990036,-1.507602
1722,-0.4206120939\C,0.9935025676,0.8328329546,-0.2381802014\C,1.30447
80813,-2.4931769528,0.4135467475\C,-0.3658193054,0.4567920063,0.325642
9288\C,1.6531718719,-1.4983736915,-1.8706882245\H,0.5785607596,-1.3039
628849,-1.94807417\H,1.8412575995,-2.4848886982,-2.3055790123\H,1.4728
564507,-3.5141493855,0.0539761469\H,0.2345177298,-2.2723405913,0.34273
8925\H,1.6059061336,-2.4355751648,1.4636086463\H,4.2132512398,-1.16998
30154,-0.9465062198\C,0.3911234689,3.2713481634,-0.3129856847\H,3.9762
83095,-1.8819528124,0.6623670915\C,2.8057653644,2.5704214386,-0.454004
4363\H,3.7572022103,-2.8829434116,-0.7937412101\H,1.515202975,2.291491
75,1.2430612311\H,2.1965017798,-0.757756667,-2.4683584824\H,0.93982375
69,0.7958014962,-1.3313142533\H,0.245884399,3.2170528221,-1.399969109\
H,0.7210391242,4.2869899892,-0.0722811328\H,-0.5798253295,3.1082317298
,0.164243703\H,2.7707036878,2.4880404752,-1.5487248636\H,3.5744669856,
1.8903839446,-0.0784256611\H,3.1043758766,3.5947262757,-0.2081032724\C
,-1.4615470838,0.3101341579,-0.5225887593\C,-2.7232763584,-0.026630749
5,-0.0210567845\C,-2.8803846797,-0.2156215535,1.3505106556\C,-1.786922
9498,-0.0735956705,2.2070366112\C,-0.535523005,0.2621478352,1.70151919
53\H,-1.3416337866,0.4711652374,-1.5941262997\C,-4.2736449679,1.216741
0141,-1.4894550479\H,-1.9151377492,-0.2277573934,3.2745073908\H,0.3221
581569,0.3570598258,2.3627886227\O,-3.8497237603,1.7150954226,-2.50339
53856\O,-5.1158538144,1.8596756233,-0.6579664837\H,-5.266578893,2.7487
135166,-1.0252277077\H,-3.8580357828,-0.4721813093,1.7506963063\C,-3.8
999774804,-0.1528474825,-0.9702042663\H,-4.7565597775,-0.5971881594,-0
.4575975842\H,-3.6349101879,-0.767407122,-1.8340731208\\Version=EM64L-
G09RevC.01\\State=2-A\\HF=-904.1726108\\S2=0.754739\\S2-1=0.\\S2A=0.750014\
RMSD=5.563e-09\\RMSF=3.048e-06\\Dipole=-0.7069113,-0.3942894,-0.2380516\
Quadrupole=1.0056297,3.6919854,-4.6976151,-0.9676753,-7.4650359,2.7397
384\\PG=C01 [X(C16H24N1O3)]\\@
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**21-P (core)**

```
1\1\GINC-R154\FOpt\RM062X\Gen\C14H19N1O3\ROOT\20-Aug-2014\0\\#M062X/ge
n 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1073741824\
\pssmtnh_core.freq\\0,1\N,-0.0353696011,-0.684288343,-0.4402537317\O,
-1.0505203442,-1.4784502247,0.1633367616\C,-2.2618866317,-0.7368716604,
0.2322507203\C,-2.1628570985,0.3866391689,1.261706368\C,-3.3741936643,
-1.6903569004,0.5681682944\C,0.2780290049,-1.327156195,-1.7107668417\C
,1.099219967,-0.7233619623,0.4850500482\C,2.224820974,0.1563768927,-0
.0038411468\H,-1.3546468776,1.0720026805,0.9910829996\H,-1.965786921,-0
.0348271431,2.2528192848\H,-2.4528394868,-0.2981312441,-0.7601012448\C
,-3.2348164269,-2.9988524654,0.7702081479\H,-2.265728093,-3.4802644721
,0.6891193774\H,1.4519544662,-1.7589420481,0.625537696\C,1.993739396,1
.5070107872,-0.2752274047\C,3.0328417704,2.3207020882,-0.7194045252\C,
4.3106237178,1.7947071406,-0.897626761\C,4.5575425868,0.4462347941,-0.
```

6354370313\c, 3.5071491334, -0.3604492412, -0.1922826424\h, 0.9928860005, 1  
 .910757257, -0.1454624857\h, 2.8485188413, 3.3710784938, -0.9251614215\c, 6  
 .9784677659, 0.4291730837, 0.1047724028\h, 3.6899260905, -1.4149522772, 0.0  
 096685368\h, 5.1224250014, 2.4358380416, -1.2308094278\o, 6.8866406622, 1.4  
 336642528, 0.7621833823\o, 8.0921299564, -0.3346262218, 0.0976385512\h, 8.7  
 380642134, 0.0909863132, 0.6887399346\c, 5.9321139095, -0.1377452523, -0.83  
 34469869\h, 6.2999423426, 0.0566183646, -1.8500590366\h, 5.9262575129, -1.2  
 257261349, -0.7164556362\h, -0.6215938364, -1.3349534981, -2.330122983\h, 0  
 .6276472575, -2.3616280933, -1.5678909947\h, 1.0528234773, -0.7435117417, -  
 2.2142059417\h, 0.7270292869, -0.3666158133, 1.4510838759\h, -3.0979042444  
 , 0.954877997, 1.3036281203\h, -4.3551928172, -1.2239527341, 0.6583585512\h  
 , -4.0899372918, -3.6186236894, 1.0223031902\\Version=EM64L-G09RevC.01\\State=1-A\\HF=-824.9553027\\RMSD=8.385e-09\\RMSF=2.371e-06\\Dipole=0.2588316  
 , -0.1401176, -0.4919636\\Quadrupole=7.499782, -3.7035516, -3.7962304, -5.64  
 56299, -2.0325223, -2.3212196\\PG=C01 [X(C14H19N1O3)]\\@

**21-P**

1\\1\\GINC-R154\\FOpt\\RM062X\\Gen\\C32H41N1O3\\ROOT\\21-Aug-2014\\0\\#M062X\\ge  
 n 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2415919104\\  
 \\pssmtnh.freq\\0,1\\N,-0.4265564065,-1.1848396221,0.6665841805\\o,0.7008  
 09619,-1.5765325772,-0.0975269519\\c,1.6883951161,-0.53461482,-0.160597  
 8505\\c,1.4977763396,0.3121624619,-1.4227508147\\c,3.0396126034,-1.21391  
 12312,-0.1359817079\\c,-0.4713718272,-3.4968855581,1.6545189805\\c,-1.50  
 52259146,-1.5526817508,-1.6211632685\\c,-0.421905873,-1.9865609461,1.92  
 28930271\\c,-1.6950189793,-1.2644695965,-0.1089947874\\c,0.8610574485,-1  
 .6571410377,2.6925467461\\c,-2.4904263927,0.0069039339,0.1586698621\\c,-  
 1.6158768167,-1.5451091234,2.7776229408\\h,-1.6111804012,-0.4588889222,  
 2.9151904347\\h,-1.5431941359,-2.0222258977,3.7604740708\\h,0.8552381384  
 ,-2.1788104796,3.6554710235\\h,0.9284505896,-0.5804322936,2.8854441676\\  
 h,1.7500326832,-1.9776177791,2.1420766832\\h,-0.4447184916,-4.045449754  
 4,2.6024480694\\c,-2.7644352083,-1.2377454454,-2.4350522103\\h,-1.384160  
 2559,-3.7916039406,1.1256220989\\c,-1.1218044977,-3.0198343379,-1.84217  
 22481\\h,0.3913556967,-3.8029554218,1.0550323093\\h,-0.6970924325,-0.916  
 295464,-1.9906830999\\h,0.4896959759,0.7468896496,-1.4063169923\\c,2.531  
 0379074,1.4371558456,-1.5934204346\\h,1.5439909267,-0.3528186083,-2.296  
 3353366\\h,1.5784039265,0.0986472088,0.7272913659\\c,4.0129703722,-0.838  
 9518205,0.7912957615\\c,5.2667582017,-1.4513181355,0.7918063913\\c,5.552  
 5514082,-2.4548198741,-0.1314565142\\c,4.5789912411,-2.8458544014,-1.05  
 19315734\\c,3.331530333,-2.2268579637,-1.0552938718\\h,3.7832971189,-0.0  
 640025798,1.5199663936\\h,6.015685763,-1.1498285376,1.5187928632\\h,6.52  
 64683302,-2.9356818339,-0.1307856738\\h,4.7929259279,-3.6352429885,-1.7  
 669364981\\h,2.5691364908,-2.5383892922,-1.7659875988\\h,3.5301608535,0.  
 9815440283,-1.6073850163\\c,2.4920614638,2.4187811883,-0.4362922349\\c,2  
 .3171627304,2.152849038,-2.9332685319\\c,3.619287753,2.6318532432,0.361  
 3448332\\c,3.5849508099,3.5251654686,1.4328227125\\c,2.4152494641,4.2235  
 185803,1.7224134549\\c,1.2857284735,4.0296655758,0.9266202989\\c,1.32689  
 44908,3.1390583477,-0.1433495523\\h,4.5341396836,2.0854971581,0.1406234  
 446\\h,4.4734525644,3.6744340177,2.0401088005\\h,2.383263283,4.917234127  
 7,2.5573725824\\h,0.3718494843,4.5778419605,1.1391562987\\h,0.4400414728  
 ,3.0061703083,-0.7609223014\\h,2.4115747576,1.4477869176,-3.7660544986\\  
 h,3.0520039797,2.9520261105,-3.0707759438\\h,1.3184186276,2.6012471633,  
 -2.9832434979\\h,-2.5787953729,-1.8298488533,2.3432012155\\h,-2.30335824  
 03,-2.1051261452,0.2590609054\\h,-3.631508111,-1.805530884,-2.075590029  
 2\\h,-2.5972414522,-1.520508947,-3.4801051798\\h,-3.0352653059,-0.179257  
 5971,-2.4074307357\\h,-1.9509203235,-3.6738273043,-1.5399888997\\h,-0.23  
 290666661,-3.3034138128,-1.2760474697\\h,-0.9291202412,-3.205007497,-2.9  
 050563262\\c,-1.858895355,1.2436886582,0.3166382949\\c,-2.6102903306,2.4  
 030770736,0.4854730454\\c,-4.0032161566,2.3413032856,0.5116997191\\c,-4.  
 6490992593,1.1110203655,0.3885335655\\c,-3.8823041559,-0.0441853871,0.2  
 226573286\\h,-0.7743053126,1.2817228773,0.3447622842\\h,-2.1088517307,3.  
 3596974973,0.6082683299\\c,-6.7679445745,0.5241524598,-0.8597777496\\h,-  
 4.386086384,-1.0048070345,0.1219194998\\h,-4.5880179293,3.2487642351,0.  
 6430001735\\o,-6.1950021388,-0.0303337589,-1.7627662196\\o,-8.0995902207  
 ,0.7481801057,-0.8760714623\\h,-8.443880528,0.3805971258,-1.7092390913\\  
 c,-6.1523826585,1.0261886585,0.4308826276\\h,-6.6035085515,1.9948379094  
 ,0.6670301748\\h,-6.4881934179,0.3351066714,1.216125213\\Version=EM64L-  
 G09RevC.01\\State=1-A\\HF=-1523.8754523\\RMSD=3.243e-09\\RMSF=1.552e-06\\Di  
 pole=-0.1911024,0.1864742,0.3983328\\Quadrupole=11.127121,-5.1945345,-5  
 .9325864,-2.5330097,0.198729,3.2717723\\PG=C01 [X(C32H41N1O3)]\\@

**21-** (core)

1\\1\\GINC-R2899\\FOpt\\UM062X\\Gen\\C10H11N1O3(1-,2)\\ROOT\\16-Aug-2014\\0\\#M

```

062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=8053
06368\\smtnc_rcore.freq\\-1,2\\N,-1.9458687359,0.6165229098,0.010750461
3\\O,-2.9392036057,0.739784019,0.8031088972\\C,-1.001853195,1.7267283976
,-0.0914388838\\C,-1.4817387068,-0.7405127125,-0.321666266\\C,-0.1767382
138,-1.0451522244,0.3730544858\\H,-1.3496342505,-0.7979128853,-1.409051
0357\\C,1.0154292598,-0.7914882767,-0.2968856635\\C,2.253597699,-0.83844
00169,0.3567645684\\C,2.2618810328,-1.2169529905,1.7024652684\\C,1.07464
95775,-1.5158550852,2.3771733903\\C,-0.1499862741,-1.4147536405,1.72308
55198\\H,0.997007916,-0.4669626874,-1.3339059855\\C,3.4505824987,1.13229
65656,-0.8116541893\\H,1.1068813357,-1.8045173323,3.4252849167\\H,-1.082
5472135,-1.5940836224,2.2543637039\\O,4.5699018309,1.6779136955,-0.8470
824497\\O,2.3239312768,1.5854916603,-1.1197783615\\H,3.2104103292,-1.256
0373527,2.2344733529\\C,3.4872537617,-0.3905837161,-0.3618579689\\H,3.61
1175673,-0.9607365222,-1.2927616327\\H,4.3832023498,-0.5520126661,0.243
9415552\\H,-0.320394678,1.584360014,-0.9341233961\\H,-0.3890307798,1.785
2262719,0.8157531031\\H,-1.5842018808,2.6423307115,-0.2066054584\\H,-2.2
939670073,-1.4041025141,-0.017637932\\Version=EM64L-G09RevC.01\\State=2
-A\\HF=-667.8556911\\S2=0.755482\\S2-1=0\\.S2A=0.750018\\RMSD=4.208e-09\\RMS
F=9.904e-06\\Dipole=-2.3809628,-2.6091945,1.0272624\\Quadrupole=-22.6434
768,6.6167585,16.0267183,-11.5861669,13.8214459,6.4518254\\PG=C01 [X(C1
0H11N1O3)]\\@
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21-

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smtnc_r      \\1\GINC-R2830\FOpt\UM062X\Gen\C16H23N1O3(1-,2)\ROOT\17-Aug-
2014\0\\#M 062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4)
maxdisk=1342          177280\\smtnc_r.freq\\-
1,2\\N,2.403144466,0.1078392319,0.0661913793\\O,3
.0091856357,0.1083391923,1.1895221158\\C,4.0568448327,-1.389948414,-0.8
666452384\\C,1.559241995,2.3746983499,0.5835351677\\C,2.5514890474,-1.12
10446791,-0.7760785684\\C,1.2420637506,1.0196016601,-0.0652601093\\C,1.8
373302906,-2.3004626623,-0.0993066443\\C,0.0021184268,0.3335820164,0.47
53457555\\C,1.9736420346,-0.8975315099,-2.1737465432\\H,0.8788573068,-0.
8739894286,-2.1767107669\\H,2.2547823401,-1.7509866797,-2.7993263225\\H,
2.1100309367,-3.2274754515,-0.616263153\\H,0.7499189086,-2.1971843461,-
0.1625256941\\H,2.1453468471,-2.3717871248,0.9491281504\\H,4.5714706194,
-0.5374927604,-1.3260109499\\C,0.3678393074,3.3176425443,0.4059710344\\H
,4.481801557,-1.5580326598,0.1258240251\\C,2.8263132027,2.9831082518,-
0.0192386278\\H,4.2280357459,-2.2767910858,-1.4852993331\\H,1.7261124365
,2.204807533,1.6535022835\\H,2.3859792479,0.0102194507,-2.6331477644\\H,
1.0979401166,1.1886198675,-1.1383472535\\H,0.1571995601,3.479905506,-0.
6595489799\\H,0.5818806439,4.2931474817,0.8575835245\\H,-0.5378393293,2.
9135460987,0.8676624196\\H,2.7091120773,3.1127951577,-1.103903675\\H,3.6
952024015,2.3448902196,0.1607163993\\H,3.0244728459,3.9700190699,0.4152
096666\\C,-1.0117071565,-0.0249876399,-0.4050394902\\C,-2.0889894152,-0.
8276939102,-0.0052276977\\C,-2.1533618934,-1.2048107563,1.338110899\\C,-
1.1669599463,-0.8069768108,2.2460895132\\C,-0.0789155548,-0.0520974566,
1.8196836945\\H,-0.9382847775,0.2465789294,-1.4550355283\\C,-2.365034175
2,-2.3140969877,-2.0966332405\\H,-1.2337561061,-1.118249104,3.286132281
6\\H,0.7274839495,0.1984394193,2.5051196012\\O,-3.1529703016,-3.12740587
54,-2.6149423337\\O,-1.1465908248,-2.1211045837,-2.3202732767\\H,-2.9724
875662,-1.8391083609,1.6713044002\\C,-3.0414841769,-1.3472429638,-1.034
706194\\H,-3.4571845135,-0.5186413256,-1.6240198629\\H,-3.881940392,-1.8
747734029,-0.5748770635\\Version=EM64L-G09RevC.01\\State=2-A\\HF=-903.63
54713\\S2=0.754806\\S2-1=0\\.S2A=0.750015\\RMSD=5.064e-09\\RMSF=4.437e-06\\D
ipole=2.8625501,3.2335925,2.2639638\\Quadrupole=-8.1576567,3.0758291,5.
0818276,-20.8503307,-21.3866512,-19.3895091\\PG=C01 [X(C16H23N1O3)]\\@
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21^-P (core)

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1\\1\GINC-R197\FOpt\RM062X\Gen\C14H18N1O3(1-)\\ROOT\22-Aug-2014\0\\#M062
X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1073741
824\\pssmtnc_core.freq\\-1,1\\N,0.1366055081,-1.3355226665,-0.406065509
5\\O,-1.0736393995,-1.7190619482,0.2443628272\\C,-1.9495487746,-0.602575
7854,0.294665056\\C,-1.4346746243,0.4756218864,1.2463135757\\C,-3.307906
0337,-1.0945731957,0.7095984456\\C,0.2237608606,-2.1498267192,-1.607853
7662\\C,1.2228431066,-1.6291309889,0.5349910237\\C,2.5547265333,-1.18090
6137,-0.0169299758\\H,-0.4596639726,0.8425389597,0.9154425304\\H,-1.3432
041116,0.065424142,2.2576080615\\H,-2.0202922759,-0.1754808619,-0.71895
4045\\C,-3.6227587869,-2.3589892381,0.9860128425\\H,-2.8808569607,-3.147
6235483,0.9128190447\\H,1.2408749528,-2.7078144002,0.7717503424\\C,3.579
1476873,-2.1026209952,-0.2505439538\\C,4.8063976276,-1.6588631418,-0.74
09952177\\C,5.0047624808,-0.3045085313,-1.00582339\\C,3.9872664405,0.635
3323324,-0.790757543\\C,2.7629264562,0.1710948927,-0.2913887594\\H,3.416
```

3126233, -3.1590633826, -0.0432860294\H, 5.6110046297, -2.3697532289, -0.91  
 54503112\C, 4.0457220086, 3.0136283195, 0.2176373101\H, 1.9857438863, 0.901  
 6733717, -0.0845292025\H, 5.9672169971, 0.0386116439, -1.3797408926\O, 2.95  
 12787377, 2.8964445301, 0.814867249\O, 5.0129569734, 3.7646835782, 0.454537  
 3539\C, 4.2047266298, 2.0965003602, -1.0603325647\H, 3.4484573141, 2.447517  
 0801, -1.775090392\H, 5.1933186309, 2.2596544182, -1.4984148544\H, -2.12693  
 00644, 1.324107054, 1.2749351034\H, -4.0633112973, -0.3128182863, 0.7951727  
 384\H, 1.1417430472, -1.8812680591, -2.1359491566\H, -0.6372977613, -1.9312  
 060523, -2.2446631785\H, 0.2367394364, -3.2273417043, -1.3723262082\H, 0.99  
 01046993, -1.086294153, 1.4564103859\H, -4.6282832047, -2.6312895451, 1.294  
 3010598\Version=EM64L-G09RevC.01\State=1-A\HF=-824.4105696\RMSD=2.665  
 e-09\RMSF=4.354e-06\Dipole=-3.9172024, -4.9646301, -1.3818569\Quadrupole  
 =-3.2036394, -17.7114839, 20.9151233, -33.6678702, -5.1643745, -9.4141945\P  
 G=C01 [X(C14H18N1O3)]\@\@

**21^-P**

1\1\GINC-R217\FOpt\RM062X\Gen\C32H40N1O3(1-)\ROOT\24-Aug-2014\0\#\M062  
 X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2415919  
 104\pssmtnc.freq\`-1,1\N,0.147568311,-1.1449962712,-0.657911989\O,-0.  
 9929855578,-1.4568877519,0.1266749454\C,-1.9367068197,-0.3703920351,0.  
 1751627384\C,-1.6842514226,0.5532670703,1.3698871447\C,-3.2986293039,-  
 1.0299020703,0.2419347882\C,-0.0230882211,-3.4714565072,-1.5999357916\  
 C,1.2104853975,-1.4871564583,1.6315920477\C,0.0635057521,-1.9662895771  
 ,-1.8972843583\C,1.4183369326,-1.3303568094,0.10371488\C,-1.1906823632  
 ,-1.5431074942,-2.669659029\C,2.353402676,-0.1777295612,-0.2230822969\  
 C,1.2849847956,-1.6548931088,-2.7695303156\H,1.3903749659,-0.574583966  
 1,-2.9109006584\H,1.1514753448,-2.1299317788,-3.748063626\H,-1.2318666  
 489,-2.0798858341,-3.6243620589\H,-1.1682204914,-0.4676528471,-2.87723  
 76885\H,-2.1007158311,-1.7800103279,-2.1108982124\H,-0.1070401259,-4.0  
 330662629,-2.5377609964\C,2.4999608234,-1.2218962631,2.4147595269\H,0.  
 8634010861,-3.8368889423,-1.0702939871\C,0.7014363411,-2.8933070238,1.  
 9685780334\H,-0.905001148,-3.6836950647,-0.9875532407\H,0.4726568841,-  
 0.7448347548,1.947637902\H,-0.6973812635,1.0257561499,1.2796478632\C,-  
 2.7422742165,1.6592295546,1.5442427115\H,-1.6665624262,-0.0569529835,2  
 .2845323133\H,-1.8501379772,0.2047736702,-0.7528769987\C,-4.2985780567  
 ,-0.7221501565,-0.6816715868\C,-5.5548688169,-1.3243211264,-0.59823124  
 19\C,-5.8195576232,-2.2523362798,0.4067029848\C,-4.820444608,-2.576682  
 1101,1.3262500495\C,-3.570782952,-1.9679557357,1.2441055416\H,-4.09135  
 66209,0.0031299551,-1.4655621598\H,-6.3244805152,-1.0692798434,-1.3221  
 332204\H,-6.7966621528,-2.7234292566,0.4727955181\H,-5.0172683582,-3.3  
 045276202,2.1090386388\H,-2.7896790171,-2.2237418353,1.956581051\H,-3.  
 7097777366,1.1789889362,1.7527901424\C,-2.9129207548,2.4922987988,0.28  
 71304479\C,-2.3585062071,2.5451913158,2.738446456\C,-4.1606296155,2.61  
 10437318,-0.3313184629\C,-4.3199891172,3.3716738041,-1.4913217425\C,-3  
 .2237088069,4.0280455697,-2.0467152627\C,-1.9765081657,3.9274528521,-1  
 .4264120459\C,-1.8176369508,3.1704397943,-0.2672995229\H,-5.016404652,  
 2.0914356957,0.0971963588\H,-5.299148469,3.4496639886,-1.9582192606\H,  
 -3.3402400888,4.6203104786,-2.9508685058\H,-1.1190987864,4.4499862716,  
 -1.8432452346\H,-0.8482162362,3.1235545554,0.2365347263\H,-2.315533967  
 9,1.9447840516,3.655577752\H,-3.0992664814,3.3399475984,2.8818136304\H  
 ,-1.3720370544,2.9981443438,2.5798588833\H,2.2181596539,-2.0302919475,  
 -2.3402389771\H,1.9162980427,-2.2611589402,-0.2154499488\H,3.313233575  
 1,-1.8758967735,2.0723968743\H,2.3276504093,-1.4296304757,3.4770928844  
 \H,2.8339366061,-0.1859496897,2.3181123174\H,1.4796793435,-3.635831419  
 3,1.7410678158\H,-0.1978430099,-3.1520214663,1.4060193454\H,0.47590736  
 22,-2.971558199,3.0391391242\C,3.7153400458,-0.4072316434,-0.440469670  
 3\C,4.5870795715,0.6690798649,-0.5907088405\C,4.1070513949,1.976998449  
 3,-0.5101734284\C,2.7449623912,2.2276784522,-0.3109155285\C,1.88173889  
 32,1.1309050596,-0.1993799663\H,4.0933818939,-1.4287328577,-0.47696463  
 95\H,5.6467467692,0.4899131413,-0.7581852785\C,1.6840746416,3.87036384  
 19,1.3152028717\H,0.8237383172,1.3167381798,-0.0530897652\H,4.79409933  
 43,2.8160504525,-0.5953973734\O,0.7025091997,3.1495591721,1.6459321539  
 \O,2.2761348169,4.7420413544,1.9719980803\C,2.2119179373,3.6230085511,  
 -0.1469745661\H,1.3623540957,3.772385244,-0.8273551367\H,2.9832560333,  
 4.3615581206,-0.3810859292\Version=EM64L-G09RevC.01\State=1-A\HF=-152  
 3.3438612\RMSD=9.476e-09\RMSF=3.431e-06\Dipole=-2.8635745,-4.7176349,-  
 2.4801703\Quadrupole=3.8796854,-18.60002,14.7203346,-19.9151937,-10.71  
 23527,-22.5592444\P G=C01 [X(C32H40N1O3)]\@\@

**22 (core)**

1\1\GINC-R850\FOpt\UM062X\Gen\C8H11B1N1O3(2)\ROOT\01-Sep-2014\0\#\M062  
 X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177

```

280\bbtnh_rcore.freq\0,2\N,-2.1810340171,-0.3100280695,-0.3704926016\
0,-2.4060408522,-0.2599951631,-1.6245153402\C,-2.1311465945,-1.6242819
477,0.2559475762\C,-1.4010039694,0.7762285499,0.2253000025\C,0.0873769
535,0.5056260184,0.1515116053\H,-1.7148556138,0.8979293635,1.267561600
8\C,0.691228839,0.2830749239,-1.0904770623\C,2.0533823028,0.0121553355
,-1.1602388302\C,2.8525012811,-0.0431316815,-0.0084025381\C,2.23139730
13,0.178742084,1.2272161087\C,0.8659345894,0.4460227672,1.3079170825\H
,0.0836186284,0.3142586716,-1.9919664165\H,2.4891915649,-0.1575831674,
-2.1442960187\B,4.3926728226,-0.3432339922,-0.0561331513\H,2.830747934
8,0.136338698,2.1326899754\H,0.4014770172,0.6114128891,2.2779916408\O,
5.0738892769,-0.399437642,1.1253802451\O,5.1029617635,-0.5535909928,-1
.2098795578\H,6.0141286126,-0.5871246596,0.9932953434\H,4.5859099824,-
0.4988085967,-2.0227295201\H,-2.952615043,-2.2157914802,-0.1486280225\
H,-2.2374615997,-1.5159606678,1.3383267775\H,-1.1764960873,-2.11710493
,0.0324659033\H,-1.6725350934,1.6740836894,-0.3352848022\\Version=ES64
L-G09RevD.01\State=2-A\HF=-616.5526411\S2=0.755147\S2-1=0.\S2A=0.75001
6\RMSD=6.978e-09\RMSF=2.923e-06\Dipole=0.3348853,-0.1458321,0.6337327\
Quadrupole=-2.0912623,0.5718221,1.5194403,0.17148,-9.7673258,-0.096525
2\PG=C01 [X(C8H11B1N1O3)]\\@
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22

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1\1\GINC-R3398\FOpt\UM062X\Gen\C14H23B1N1O3(2)\ROOT\14-Aug-2014\0\\#M0
62X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=10737
41824\bbtnh_r.freq\0,2\N,-2.1338882415,-0.3178769663,-0.3802755378\O,
-2.2422601597,-0.260843801,-1.6491403461\C,-3.6815559591,-2.1799017034
,-0.2553001969\C,-1.78322599,2.1277207026,-0.3280756391\C,-2.329892112
1,-1.660431943,0.2412364718\C,-1.3792600594,0.770298133,0.2755955278\C
,-1.1998164152,-2.5917068648,-0.217504704\C,0.1131813526,0.5010293595,
0.1984538561\C,-2.345870059,-1.5507143967,1.7649332915\H,-1.3723148345
,-1.252738466,2.1674150334\H,-2.5866001502,-2.5336167159,2.1815732088\H
,-1.3946595499,-3.6100580947,0.1359868741\H,-0.2315763347,-2.26729558
1,0.1772034329\H,-1.1486055592,-2.6022643952,-1.3102531904\H,-4.487700
561,-1.5056561103,0.0538411324\C,-1.0278576972,3.25617421,0.3763941726
\H,-3.6877094913,-2.2510808436,-1.3447398105\C,-3.2943352368,2.3334214
908,-0.2160334637\H,-3.8721176194,-3.1710308578,0.1683758124\H,-1.5051
026905,2.1152110942,-1.3882331099\H,-3.109713287,-0.8434563794,2.10752
02203\H,-1.6778623725,0.7797310742,1.3292496811\H,-1.2484360438,3.2617
926245,1.452144544\H,-1.3343537183,4.2254760298,-0.0295043809\H,0.0555
560576,3.164765161,0.2545558464\H,-3.6107467379,2.2933064385,0.8350600
201\H,-3.8438937542,1.5710681437,-0.7737551484\H,-3.5755264785,3.31570
68036,-0.6096114837\C,0.7291080349,0.274008128,-1.0368672076\C,2.09572
29234,0.0228825116,-1.0954796243\C,2.8909557291,-0.0070080696,0.059895
607\C,2.2604402578,0.22863197,1.2887213745\C,0.8914465777,0.4781225173
,1.3574754962\H,0.1260827362,0.2733769432,-1.9416169239\H,2.5379027804
,-0.1563451838,-2.0752462867\B,4.4333752077,-0.2919416272,0.022900057\
H,2.8559334515,0.2121635491,2.1977015137\H,0.4206856444,0.6589921259,2
.3225338653\O,5.1149571769,-0.310429036,1.2058633018\O,5.1474125827,-0
.5256168926,-1.1246192676\H,6.0567107069,-0.4930745911,1.0779502972\H
,4.6276158938,-0.5011374912,-1.9372803171\\Version=EM64L-G09RevC.01\Sta
te=2-A\HF=-852.3315446\S2=0.754739\S2-1=0.\S2A=0.750014\RMSD=5.136e-09
\RMSF=7.952e-06\Dipole=0.0431174,-0.1675232,0.4696703\Quadrupole=-0.42
13519,0.334213,0.0871388,0.0232488,-7.331933,-0.661552\PG=C01 [X(C14H2
3B1N1O3)]\\@
```

22-P (core)

```

1\1\GINC-R94\FOpt\RM062X\Gen\C12H18B1N1O3\ROOT\16-Aug-2014\0\\#M062X/g
en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1073741824
\psbtanh_core.freq\0,1\N,-0.1302528317,-0.9152038478,0.5479537223\O,1
.1176804757,-1.4985159268,0.1908195272\C,2.1121288356,-0.4789937186,0.
0586337597\C,1.8276860025,0.4091360141,-1.1485028664\C,3.4204775841,-1
.2022670231,-0.0823342705\C,-0.4326486049,-1.4004763783,1.8894089453\C
,-1.0947153306,-1.4065976135,-0.4376646759\C,-2.4543181349,-0.78621818
86,-0.2218793184\H,0.8450483909,0.8787342101,-1.0468732026\H,1.8453239
189,-0.1870551433,-2.0677590046\H,2.1184719672,0.1264981248,0.97642734
6\C,4.4904640024,-0.9574474727,0.6699976922\H,4.4627381315,-0.22282194
32,1.4720069562\H,-1.1625542021,-2.5069264342,-0.4033582007\C,-2.59039
76604,0.6050995708,-0.1509843901\C,-3.8408675628,1.1824619434,0.035459
3209\C,-4.997218993,0.3942340602,0.1557206079\C,-4.8453841217,-0.99499
44719,0.0859247773\C,-3.5935262954,-1.5811435578,-0.0958975154\H,-1.70
25402673,1.227246354,-0.2322315685\H,-3.9364365723,2.2636867711,0.0896
539368\B,-6.3897277433,1.0869978955,0.3614073911\H,-5.7086941996,-1.65
34332608,0.1790647477\H,-3.500133997,-2.6639006456,-0.1390174949\O,-6.
```

```

4288718911,2.4495931363,0.4349027703\O,-7.5791899013,0.4119976281,0.47
22655046\H,-7.3301191509,2.779576555,0.5593139634\H,-7.5075100565,-0.5
481180726,0.4089990213\H,2.5859758896,1.1938646268,-1.2284182952\H,3.4
596405948,-1.9455439448,-0.8790496718\H,-1.3878049668,-0.9746013548,2.
2071972981\H,0.3520461733,-1.0614149532,2.5690473958\H,-0.487838932,-2
.4996506202,1.9208516315\H,-0.7044816001,-1.1295899877,-1.422904906\H,
5.4301810493,-1.4776323308,0.5116090654\\Version=EM64L-G09RevC.01\Stat
e=1-A\HF=-773.1141922\RMSD=4.350e-09\RMSF=2.326e-06\Dipole=-0.1512081,
-0.3274216,0.0615525\Quadrupole=4.2289977,-1.2498806,-2.9791172,5.1738
011,-0.3407455,0.9002847\PG=C01 [X(C12H18B1N1O3)]\\@
```

**22-P**

```

1\1\GINC-R3084\FOpt\RM062X\Gen\C30H40B1N1O3\ROOT\17-Aug-2014\0\\#M062X
/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=21474836
48\psbttnh.freq\\0,1\N,0.2675770316,-1.4310993819,-0.907987218\O,1.250
0849431,-0.5456966585,-1.4154974359\c,1.7866696023,0.30154687,-0.38436
15387\c,1.0645737687,1.6526822431,-0.3727839232\c,3.2644915165,0.45647
75419,-0.6673712008\c,1.2162143352,-3.2397016604,-2.3747673931\c,-1.12
09528779,-0.0752401367,-2.5680533916\c,0.8267114348,-2.8113205396,-0.9
536101765\c,-1.0466652465,-1.2747911437,-1.588647713\c,2.0705024609,-2
.8491118266,-0.0603474575\c,-2.1263067724,-1.2370835735,-0.5146104858\
c,-0.214772631,-3.7675436139,-0.3601838221\H,-0.537998965,-3.421026922
,0.6268881496\H,0.2359028831,-4.7594457263,-0.2518763534\H,2.458359922
,-3.8722361305,-0.0147261217\H,1.8224523449,-2.5299061978,0.9582508792
\H,2.8631182881,-2.2060294358,-0.452532447\H,1.6418833027,-4.248967307
9,-2.3571996086\c,-2.5643467619,0.2770097259,-2.9402902049\H,0.3547000
295,-3.2543210503,-3.0512516401\c,-0.3343533128,-0.3762373386,-3.84787
40166\H,1.967210268,-2.5563651351,-2.7830078748\H,-0.6783402974,0.7949
217881,-2.0769175994\H,-0.0064505877,1.4796105664,-0.2052715284\c,1.58
37610697,2.6407788238,0.6841107599\H,1.1627212577,2.1059202509,-1.3691
973345\H,1.646257414,-0.2005236467,0.5798267543\c,4.2148894825,0.18512
93837,0.318054375\c,5.5752144008,0.3555104424,0.0589046046\c,5.9965854
703,0.7892379579,-1.196354705\c,5.0531014409,1.0478863516,-2.191660805
7\c,3.6955831696,0.8849786473,-1.9270516831\H,3.8844717866,-0.16702705
98,1.2933027582\H,6.3046148291,0.141150896,0.834967816\H,7.0551731894,
0.9192986881,-1.4017073739\H,5.3769555385,1.3762314977,-3.1752445908\H
,2.9607984306,1.0774811503,-2.705769327\H,2.6581083889,2.7898187722,0.
5122108792\c,1.4159046197,2.0968378684,2.0915580608\c,0.8861892653,3.9
978488941,0.526824985\c,2.5247450816,1.8880985099,2.9157405922\c,2.376
6365601,1.3782010086,4.2062615069\c,1.1089920029,1.0704437405,4.694164
0508\c,-0.0086137626,1.2859013317,3.8870479414\c,0.1456377697,1.796734
7284,2.6004449858\H,3.5169932926,2.127064019,2.5381996607\H,3.25316411
05,1.2233757589,4.8294093895\H,0.9894599788,0.6711683041,5.696998157\H
,-1.0024964782,1.059754914,4.2637073537\H,-0.7378465643,1.9679694211,1
.9872962089\H,1.0707805991,4.4126844196,-0.4699121049\H,1.2496907518,4
.7119548375,1.272045823\H,-0.1976870446,3.8997368105,0.6555839758\H,-1
.1019016458,-3.876802819,-0.9912018568\H,-1.2480387999,-2.1578093128,-
2.2148180846\H,-3.0802768986,-0.5820088008,-3.3882809404\H,-2.56147374
02,1.0818680387,-3.683099826\H,-3.1503929538,0.6094732696,-2.079367309
3\H,-0.8028113488,-1.2082496872,-4.3908008757\H,0.7035948636,-0.640111
1859,-3.6387978465\H,-0.3427734472,0.495654449,-4.5117803266\c,-1.9137
728258,-0.5863533049,0.7035329374\c,-2.9270793154,-0.5078989658,1.6537
623343\c,-4.1826260583,-1.0933128215,1.4346345206\c,-4.3730954467,-1.7
714766265,0.223179505\c,-3.3650130371,-1.8453914546,-0.7340976527\H,-0
.931619527,-0.1757672527,0.9170074213\H,-2.7445182556,0.0043939667,2.5
953994042\B,-5.2923944716,-0.9878547079,2.5356452152\H,-5.3200715312,-
2.2659184815,0.0069143025\H,-3.5405269641,-2.3851188193,-1.6631457123\
0,-4.9981851247,-0.3247134482,3.6935953493\O,-6.552516639,-1.519116440
4,2.4156687508\H,-5.7495427291,-0.3160865913,4.3034418056\H,-6.7189818
335,-1.9730826822,1.5806202938\\Version=EM64L-G09RevC.01\State=1-A\HF=
-1472.0343965\RMSD=1.661e-09\RMSF=3.503e-06\Dipole=0.0691889,-0.254560
6,-0.3699219\Quadrupole=6.290284,-5.0615244,-1.2287596,5.128244,3.7040
587,-1.172864\PG=C01 [X(C30H40B1N1O3)]\\@
```

**22-** (core)

```

1\1\GINC-R848\FOpt\UM062X\Gen\C8H12B1N1O4(1-,2)\ROOT\01-Sep-2014\0\\#M
062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342
177280\\btnc_rcore.freq\\-1,2\N,-2.5139066353,-0.3565314312,-0.2789814
307\O,-3.1195856658,-0.3147638015,-1.4018707442\c,-2.1530530514,-1.662
215718,0.2527727857\c,-1.7527610108,0.8198437271,0.1727994682\c,-0.260
9677071,0.5948849564,0.1250444972\H,-2.0627660245,1.049258233,1.201406
8831\c,0.388108591,0.4009282356,-1.1007127707\c,1.7554476313,0.1374591
```

822,-1.1333036625\c,2.5357589875,0.0518591347,0.0339749801\c,1.8641210  
 899,0.2570943126,1.2460942533\c,0.4917635968,0.5189335563,1.2975342465  
 \h,-0.1926215192,0.4500717301,-2.0225463228\h,2.2514355139,-0.00178977  
 81,-2.0931043973\b,4.1438426005,-0.3083117798,-0.0478232143\h,2.444455  
 2069,0.2070855366,2.1650385626\h,-0.0035415018,0.6671981975,2.25894221  
 63\o,4.7235387992,0.031882989,1.2624941643\o,4.357644335,-1.7345883314  
 ,-0.3604197917\h,5.5401441401,-0.4799910274,1.3293372991\h,4.737496425  
 7,-1.7617394697,-1.2476801519\o,4.7845006012,0.4450767175,-1.164712663  
 1\h,4.8714750593,1.365251501,-0.8875754606\h,-2.9922183864,-2.33614024  
 27,0.0737330006\h,-1.9502724075,-1.573389892,1.3235272092\h,-1.2505936  
 738,-2.0405787429,-0.242211091\h,-2.0807749947,1.6291222052,-0.4842478  
 656\Version=ES64L-G09RevD.01\State=2-A\HF=-692.4178259\S2=0.755475\S2  
 -1=0.\S2A=0.750018\RMSD=4.166e-09\RMSF=2.589e-06\Di pole=-2.7251119,0.3  
 319953,0.7033825\Quadrupole=-24.9011832,13.5937045,11.3074787,3.03093,  
 -9.5408591,-0.2921341\PG=C01 [X(C8H12B1N1O4)]\@\n

**22-**

1\1\GINC-R993\FOpt\UM062X\Gen\C14H24B1N1O4(1-,2)\ROOT\15-Aug-2014\0\#\n
 M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=134  
 2177280\btnc\_r.freq\~-1,2\N,-2.2379773734,-0.2865997276,-0.344925201\o,  
 -2.4888813119,-0.1909701429,-1.5925924272\c,-3.6307494841,-2.2626172  
 505,-0.1767133029\c,-1.9113040995,2.1601524424,-0.2934900781\c,-2.2799  
 988419,-1.663452726,0.226943476\c,-1.4606306039,0.8091511183,0.2869620  
 065\c,-1.1341053893,-2.4993540042,-0.3601003915\c,0.0296065657,0.55556  
 65213,0.1721540779\c,-2.176368674,-1.6139993354,1.7509377075\h,-1.1979  
 376513,-1.252772719,2.0798144816\h,-2.305407534,-2.6292682479,2.140926  
 9415\h,-1.2516523673,-3.5460764836,-0.0551290343\h,-0.1588762731,-2.14  
 06207,-0.0191379532\h,-1.1606508194,-2.4447919576,-1.4526118921\h,-4.4  
 531361353,-1.6531932009,0.2157826877\c,-1.1290547003,3.2928764346,0.37  
 31889205\h,-3.7200397052,-2.3051750577,-1.2642251401\c,-3.4163886922,2  
 .3621888433,-0.1076506802\h,-3.7183187123,-3.2757082125,0.2303830429\h  
 ,-1.6836563161,2.1517667501,-1.3655014126\h,-2.9610343062,-0.981447494  
 3,2.1831433299\h,-1.7310551371,0.808723094,1.3507259125\h,-1.298574393  
 1,3.2959423843,1.4587769696\h,-1.4566768163,4.2623674687,-0.0194019613  
 \h,-0.0536021211,3.1931771258,0.2034146167\h,-3.6779685719,2.322501201  
 3,0.9592431419\h,-3.9893869442,1.5946676578,-0.6343230975\h,-3.7232904  
 112,3.3437350123,-0.4875234941\c,0.6350290258,0.3720612314,-1.07690881  
 93\c,2.0043122502,0.1266130664,-1.1589824556\c,2.8296572495,0.04914031  
 01,-0.0229399818\c,2.2019075569,0.2520615135,1.2131609841\c,0.82938885  
 42,0.4986089765,1.3145316186\h,0.0192105841,0.397889224,-1.9758297482\h  
 ,2.4639187717,-0.0120534113,-2.136856999\b,4.4361355853,-0.2971230844  
 ,-0.1660039657\h,2.8162842195,0.211108509,2.110205761\h,0.3707236375,0  
 .6512569815,2.2939481348\o,5.0605367653,0.0396619986,1.1250789862\o,4.  
 6493931889,-1.7190700305,-0.4978631038\h,5.8805665764,-0.4696669619,1.  
 1619857434\h,5.0123938984,-1.7347870979,-1.3924224396\o,5.0303790145,0  
 .4700648871,-1.2990530005\h,5.1280666419,1.3868530942,-1.0144299616\Version=EM64L-G09RevC.01\State=2-A\HF=-928.195504\S2=0.754818\S2-1=0.\S2A=0.750015\RMSD=5.139e-09\RMSF=3.070e-06\Di pole=-5.0342644,0.42785,0.  
 8533985\Quadrupole=-34.2115746,17.6320948,16.5794798,6.2145971,-4.6127  
 955,-0.7522852\PG=C01 [X(C14H24B1N1O4)]\@\n

**22^-P (core)**

1\1\GINC-R2036\FOpt\RM062X\Gen\C12H19B1N1O4(1-)\ROOT\19-Aug-2014\0\#\n
 M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1073  
 741824\psbtnc\_core.freq\~-1,1\N,-0.1954618135,-0.9698408936,-0.286823  
 6666\o,-1.4498466574,-1.5279563053,0.1171030324\c,-2.4466847106,-0.524  
 5531997,0.0585920722\c,-2.2346136329,0.534516134,1.1397256342\c,-3.790  
 052478,-1.1847938625,0.1988715132\c,0.1521830696,-1.6283215123,-1.5382  
 92882\c,0.7551684089,-1.2953488564,0.7880340009\c,2.1345628239,-0.7742  
 263287,0.4767059791\h,-1.2550238615,1.0013499043,1.0072436551\h,-2.282  
 9901737,0.0679080551,2.1292923483\h,-2.3924950633,-0.0362735492,-0.928  
 5581701\c,-3.994105734,-2.4914107464,0.3569864654\h,-3.1608382726,-3.1  
 861741225,0.3827422433\h,0.7813846342,-2.388000359,0.9428937198\c,2.37  
 68076098,0.6016256965,0.4086177801\c,3.646208177,1.0832473318,0.088454  
 9309\c,4.7279668084,0.2263745519,-0.1734993677\c,4.4596681641,-1.14870  
 35667,-0.1041555576\c,3.1943991116,-1.6461349788,0.2138337763\h,1.5546  
 245991,1.2926149119,0.5986513574\h,3.8219873019,2.1554988916,0.0302949  
 074\b,6.245622925,0.7834427603,-0.503798359\h,5.2722078477,-1.84252706  
 34,-0.3168125691\h,3.0199364558,-2.7223925018,0.2552665529\o,6.9110629  
 029,-0.0973968064,-1.5086871045\o,7.1081176339,0.7410896645,0.69386088  
 45\h,6.5304895627,0.1063697224,-2.3716520456\h,7.7584200169,0.04591355  
 66,0.532689562\o,6.0991314848,2.1677802456,-0.9841149433\h,6.955604116

```
,2.5884454776,-0.8321684424\H,-4.6368122843,-0.4976813512,0.1798219847
\H,-4.9978998079,-2.8927744486,0.4645157284\H,-3.0052592973,1.31114460
7,1.0780800162\H,-0.6260464484,-1.4129974891,-2.2755921646\H,0.2431400
351,-2.7198480136,-1.4138412743\H,1.1047229529,-1.2216998781,-1.884455
9629\H,0.3518635932,-0.8386856777,1.6990443651\\Version=EM64L-G09RevC.
01\State=1-A\HF=-848.9768325\RMSD=3.718e-09\RMSF=2.533e-06\Dipole=-5.9
429413,-1.4829187,0.013317\Quadrupole=-36.7547986,16.9262664,19.828532
2,-19.1527717,2.9340281,0.9841998\PG=C01 [X(C12H19B1N1O4)]\\@
```

**22^-P**

```
1\1\GINC-R2217\FOpt\RM062X\Gen\C30H41B1N1O4(1-) \ROOT\20-Aug-2014\0\\#M
062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2415
919104\psbtnc.freq\\-1,1\N,-0.0523858249,-1.6553346124,0.4881142173\O
,1.1997841221,-1.6781747838,-0.1821076271\C,1.7994863138,-0.3743871336
,-0.2026013357\C,1.4752206875,0.3492921696,-1.5145139732\C,3.289060566
6,-0.5734435833,-0.0265187029\C,0.4993235254,-3.8761928135,1.528751929
6\C,-0.7927923313,-2.3390068813,-1.8533823256\C,0.0909212049,-2.412899
0807,1.755906854\C,-1.1916633838,-2.0836900641,-0.3777262154\C,1.16339
60102,-1.7227606304,2.6064272587\C,-2.3172607924,-1.0726049277,-0.2108
521467\C,-1.2409577865,-2.3286666921,2.5117995066\H,-1.56314026,-1.287
0300033,2.6053948666\H,-1.1072487232,-2.7534529511,3.5131780545\H,1.23
69777635,-2.2197682059,3.5803392696\H,0.8985090643,-0.672837818,2.7748
236798\H,2.14581354,-1.7703010017,2.1272342779\H,0.6094435459,-4.38950
42351,2.4912535889\C,-2.0195325234,-2.4220497096,-2.7657235076\H,-0.24
91629884,-4.4199907393,0.9425266141\C,0.0204272134,-3.6312207457,-1.98
85065406\H,1.4569905358,-3.923773907,0.9998841688\H,-0.1801449645,-1.5
010224685,-2.1957308651\H,0.3849688893,0.4280418552,-1.6056261584\C,2.
0970829889,1.7490276093,-1.646233483\H,1.8230376881,-0.2776978756,-2.3
481107328\H,1.4005300748,0.2014495035,0.6404402244\C,4.0027185871,0.15
1458692,0.9293505523\C,5.3811652667,-0.0162648006,1.0661272884\C,6.058
1597479,-0.9225139082,0.2523097261\C,5.3492176784,-1.6621750558,-0.695
7565027\C,3.974569304,-1.4863865134,-0.8350103903\H,3.4696276983,0.849
5675891,1.5715119841\H,5.9234333202,0.5556036117,1.8144630589\H,7.1309
596442,-1.0577874426,0.3594565489\H,5.86950508124,-2.378236636,-1.32634
5082\H,3.4177940846,-2.0692324175,-1.565427571\H,3.1872917287,1.651009
8926,-1.5477129335\C,1.6220097651,2.6924706216,-0.5550004749\C,1.79639
09157,2.3258797342,-3.0359851935\C,2.5358662772,3.3020215961,0.3092397
425\C,2.1051944885,4.1637526697,1.3190556547\C,0.7464418441,4.42759305
12,1.4780546934\C,-0.1769507935,3.8357474488,0.6150920711\C,0.26063193
52,2.9823184905,-0.3953800304\H,3.5976522899,3.0919912376,0.191046496\
H,2.8326616119,4.6249784959,1.9823958665\H,0.4052174362,5.0896624034,2
.2688479974\H,-1.2398525025,4.0305012917,0.7291613576\H,-0.4767651023,
2.5324213572,-1.0574966676\H,2.1956856159,1.6728145725,-3.8201932635\H
,2.2413747907,3.3196474509,-3.1503011632\H,0.7161466217,2.4203084558,-
3.1923008501\H,-2.0447350008,-2.8809446241,2.0172885761\H,-1.569604614
6,-3.0578287966,-0.0255244987\H,-2.6996953671,-3.2197714535,-2.4403034
669\H,-1.6990385431,-2.6536593452,-3.7886472439\H,-2.5879460171,-1.489
2352484,-2.7786414426\H,-0.5970938746,-4.4944336949,-1.7034032615\H,0.
9129550944,-3.6230110173,-1.3594425433\H,0.3317259383,-3.7801733258,-3
.0298981825\C,-2.0543221978,0.2904957972,-0.066581707\C,-3.096535202,1
.2171055883,0.0056807652\C,-4.4446168533,0.8366099316,-0.0389117304\C,
-4.6871008857,-0.5432752668,-0.1388503391\C,-3.6555724022,-1.479318244
9,-0.2240161116\H,-1.0226093775,0.6152045525,0.0400887307\H,-2.8748056
88,2.2766974735,0.1219695807\B,-5.6803364093,1.9267923954,0.0215390699
\H,-5.7212688854,-0.8864552692,-0.1358083039\H,-3.8891516261,-2.543265
4976,-0.3004882263\O,-6.7580364592,1.438382073,0.9307693906\O,-6.32492
70404,2.0930851604,-1.2955349017\H,-6.4295453849,1.4950699677,1.836353
2022\H,-7.2057060573,1.705868083,-1.2153322968\O,-5.0957991824,3.20170
09374,0.4773948664\H,-5.7197701859,3.887167662,0.2050392621\\Version=EM
64L-G09RevC.01\State=1-A\HF=-1547.8962267\RMSD=7.697e-09\RMSF=1.866e-
06\Dipole=7.7127235,-2.2734354,0.3366242\Quadrupole=-51.3284978,18.181
8756,33.1466222,27.7260212,-2.2110632,4.0411496\PG=C01 [X(C30H41B1N1O4
)]\\@
```

**23 (core)**

```
1\1\GINC-R851\FOpt\UM062X\Gen\C9H13B1N1O3(2) \ROOT\01-Sep-2014\0\\#M062
X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177
280\\sbtnc_rcore.freq\\0,2\N,-2.5080465084,-0.0806565884,-0.4344653021
\O,-2.6372729227,0.0385637412,-1.6974152323\C,-2.7388035288,-1.3961322
938,0.1469927518\C,-1.5801118647,0.8281565939,0.242260449\C,-0.1657613
323,0.2883086671,0.2466019116\H,-1.9320254901,0.9820704786,1.268146159
6\C,0.4767305319,0.0021713753,-0.9627969473\C,1.7658939072,-0.52137622
```

```

98,-0.9666323455\C,2.4545733865,-0.7746248639,0.23018795\C,1.803531193
7,-0.4839780436,1.4320875533\C,0.5080535005,0.0335809422,1.4402769858\
H,-0.0477670501,0.1789698699,-1.8992833228\H,2.2490927263,-0.747003505
3,-1.9159087695\B,4.9375372605,-0.1462369635,-0.1530230725\H,2.3133429
897,-0.672118564,2.3742071697\H,0.0191769952,0.2423772846,2.3898319212
\O,6.2631400404,-0.459916095,-0.0745435583\O,4.5903956022,1.11775666,-
0.5429644396\H,6.8265086704,0.288444423,-0.3204354345\H,3.6319656546,1
.2590614051,-0.5664823487\C,3.8744217413,-1.2749806885,0.2040556033\H,
3.9834512535,-2.0791196351,-0.5363010731\H,4.1501721022,-1.7201998142,
1.1673318685\H,-3.6255292206,-1.8171154687,-0.3272448812\H,-2.89500762
06,-1.2959029402,1.2241465665\H,-1.876834833,-2.0501582379,-0.03583255
88\H,-1.6489671848,1.773088491,-0.3021976042\Version=ES64L-G09RevD.01
\State=2-A\HF=-655.8472965\S2=0.755152\S2-1=0.\S2A=0.750015\RMSD=6.560
e-09\RMSF=2.949e-06\Di pole=0.0233089,-0.0562242,1.0929321\Quadrupole=-
3.5635747,1.5821213,1.9814534,3.5916088,-9.8007082,0.9588435\PG=C01 [X
(C9H13B1N1O3)]\\@
```

23

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1\1\GINC-R393\FOpt\UM062X\Gen\C15H25B1N1O3(2)\ROOT\15-Aug-2014\0\\#M06
2X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=134217
7280\sbtnh_r.freq\0,2\N,-2.0068767829,-0.3130161612,-0.4054392978\O,
-1.9269949744,-0.2170916177,-1.6742039164\C,-3.6167357686,-2.118582613
6,-0.566982084\C,-1.5893102394,2.1144578256,-0.2220298076\C,-2.3351910
718,-1.6641140456,0.1363059119\C,-1.3168191875,0.7266858008,0.38642149
4\C,-1.1820104996,-2.6241958858,-0.1852271393\C,0.1615266198,0.4040503
424,0.5109270517\C,-2.5693625517,-1.5962618314,1.6444273693\H,-1.65512
36218,-1.3475950929,2.1929674073\H,-2.9021959565,-2.5800871289,1.98931
54163\H,-1.4599154375,-3.6440828924,0.1021393725\H,-0.2711987164,-2.34
76280036,0.3555183602\H,-0.9725875431,-2.605965651,-1.258817075\H,-4.4
366112941,-1.4235214496,-0.3554087238\C,-0.9126714245,3.1949617541,0.6
233335704\H,-3.4667328229,-2.1590641966,-1.6476336656\C,-3.0936957264,
2.3693996859,-0.3235003095\H,-3.899430007,-3.1133224767,-0.2081850778\H,
-1.1599395333,2.1246848452,-1.2306025391\H,-3.349933076,-0.869293002
4,1.8960500431\H,-1.7615457374,0.7168752688,1.3874178656\H,-1.29177279
53,3.1791322072,1.6538790047\H,-1.1225338921,4.1859239655,0.2084465892
\H,0.1732977606,3.0665926844,0.662231587\H,-3.5621274445,2.3056041274,
0.6680129654\H,-3.5776342399,1.6453526107,-0.9835727471\H,-3.285020816
8,3.3732887207,-0.7165620838\C,0.943506774,0.1927274378,-0.6296302344\
C,2.2966233053,-0.1102450369,-0.5087865139\C,2.9150252481,-0.209593217
8,0.7472607246\C,2.1271334131,0.0124178662,1.8801470181\C,0.7695369985
,0.3107699894,1.762712785\H,0.4782737618,0.2412183178,-1.6114316269\H,
2.8870081048,-0.2861368391,-1.4067785962\B,5.2879356355,0.8009694568,0
.5224006883\H,2.5798468912,-0.0545747926,2.8669080311\H,0.1765869486,0
.4751062562,2.6611133773\O,6.6357531362,0.7143053475,0.7186652393\O,4.
7753627587,1.9745202958,0.0422822099\H,7.0884996737,1.5364220946,0.479
7832056\H,3.8120208854,1.9516999185,-0.0624856433\C,4.3938935341,-0.47
24893156,0.8541263914\H,4.6911486027,-1.2751279909,0.165488432\H,4.656
3701093,-0.8306105771,1.8566569704\Version=EM64L-G09RevC.01\State=2-A
\HF=-891.6260271\S2=0.754732\S2-1=0.\S2A=0.750014\RMSD=3.189e-09\RMSF=
3.793e-06\Di pole=-0.3389877,-0.0610107,0.8769135\Quadrupole=-2.4862156
,2.5220051,-0.0357895,2.8459036,-6.4088527,-0.6188836\PG=C01 [X(C15H25
B1N1O3)]\\@
```

23-P (core)

```

1\1\GINC-R3118\FOpt\RM062X\Gen\C13H20B1N1O3\ROOT\19-Aug-2014\0\\#M062X
/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=10737418
24\pssbt nh_core.freq\0,1\N,-0.1089281311,-0.9087866031,-0.2640338601
\O,-1.3920652151,-1.4821199479,-0.04066348\C,-2.368150291,-0.452321624
4,0.054944113\C,-2.2078024482,0.3409126937,1.3499016116\C,-3.727199055
6,-1.0884112868,-0.0324743228\C,0.2912843869,-1.3267180807,-1.60222037
36\C,0.7624368465,-1.4750871471,0.7681432447\C,2.1450703865,-0.8736387
392,0.6979205393\H,-1.2165214921,0.8016664761,1.386445888\H,-2.3314595
266,-0.3246831696,2.2104106532\H,-2.234598388,0.2280803861,-0.80116696
12\C,-3.9621031517,-2.3913293109,-0.1722726034\H,-3.1478892426,-3.1047
391922,-0.2468417217\H,0.8149621242,-2.5729469037,0.6755920305\C,3.278
6828896,-1.6764369559,0.577165837\C,4.553449485,-1.1100599797,0.531133
8245\C,4.731394405,0.2764825651,0.5979287711\C,3.5863115064,1.07713821
46,0.7067705122\C,2.3157103755,0.5132904712,0.75964274\H,3.1674805856,
-2.7572173501,0.5225151135\H,5.4253026403,-1.7570218889,0.4480788426\B
,6.6521458128,0.9134946471,-1.0163954346\H,3.697221503,2.1581522021,0.
7560238811\H,1.4386020105,1.150882207,0.8397233898\O,7.8244722614,1.56
64530823,-1.2651278316\O,6.0108100528,0.3074656344,-2.0616889377\H,8.0
```

72933608, 1.5182060668, -2.1998776661\H, 5.1852998861, -0.1248959311, -1.79  
 49425208\C, 6.1050220923, 0.882544406, 0.4769247106\H, 6.8273463975, 0.3193  
 933915, 1.0834424193\H, 6.1181081408, 1.9040953594, 0.8749312305\H, -2.9596  
 20898, 1.1345640645, 1.4116228339\H, -4.558173487, -0.3873802205, 0.0450910  
 206\H, -4.9773604494, -2.773755941, -0.214919412\H, -0.4326197748, -0.93769  
 25394, -2.3215747269\H, 0.3352724487, -2.4234738969, -1.6901339289\H, 1.273  
 961624, -0.9009539526, -1.8203429555\H, 0.2933700817, -1.2468212061, 1.7309  
 7353\\Version=EM64L-G09RevC.01\\State=1-A\\HF=-812.4093287\\RMSD=5.086e-0  
 9\\RMSF=5.253e-06\\Dipole=-0.2192526, -0.0040823, -0.1114426\\Quadrupole=-1  
 .9158042, 2.4867424, -0.5709382, -6.3182682, -1.5036221, 0.1281379\\PG=C01 [  
 X(C13H20B1N1O3)]\\@

**23-P**

1\\1\\GINC-R3081\\FOpt\\RM062X\\Gen\\C31H42B1N1O3\\ROOT\\21-Aug-2014\\0\\#M062X  
 /gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=24159191  
 04\\pssbt nh.freq\\0,1\N, -0.1899604169, -1.5261924602, 0.5365863341\O, 1.0  
 70960502, -1.6153715544, -0.1039633193\C, 1.7438808139, -0.3451666453, -0.1  
 310637076\C, 1.4724458235, 0.3796840087, -1.4530535731\C, 3.2171275123, -0.  
 6267399965, 0.0645219224\C, 0.2757193724, -3.742317409, 1.631297321\C, -0.8  
 937565841, -2.232563163, -1.8140949322\C, -0.0976665447, -2.2665967777, 1.8  
 267385049\C, -1.3085823657, -1.9615279045, -0.3451946405\C, 0.9730659792, -  
 1.5896470189, 2.6880931365\C, -2.4303317752, -0.939381562, -0.212947201\C,  
 -1.4428257255, -2.136207471, 2.5510032762\H, -1.7314122724, -1.0835033673,  
 2.6389762662\H, -1.3458129388, -2.556322235, 3.5573736306\H, 1.0074231638,  
 -2.0673260088, 3.6729306137\H, 0.7395171056, -0.5282061826, 2.8292629897\H  
 , 1.9646165953, -1.6796100224, 2.2359318616\H, 0.3555243218, -4.2390416919,  
 2.6044112197\C, -2.1029227122, -2.2917420023, -2.7523039413\H, -0.47383823  
 34, -4.2828182441, 1.0432255516\C, -0.1152509496, -3.5480226694, -1.9201659  
 333\H, 1.2413061964, -3.8240263354, 1.1230102627\H, -0.2508821708, -1.41317  
 16326, -2.1456134025\H, 0.3889253514, 0.5170349835, -1.5650494891\C, 2.1681  
 108853, 1.7445286441, -1.5804880375\H, 1.798485111, -0.2689847213, -2.27800  
 90556\H, 1.3703726735, 0.259511092, 0.7033552476\C, 3.9420076333, 0.0156495  
 338, 1.0694161705\C, 5.3064492416, -0.2290838189, 1.2282227765\C, 5.9552911  
 64, -1.1303572246, 0.386898725\C, 5.2339216248, -1.7884003703, -0.610304404  
 7\C, 3.8740159359, -1.5355364154, -0.7714830434\H, 3.4306143424, 0.70886019  
 34, 1.7344375182\H, 5.8589588069, 0.2780148611, 2.0142363196\H, 7.016621790  
 3, -1.3251697655, 0.5105253231\H, 5.7326764375, -2.5002023789, -1.261972658  
 8\H, 3.3100848629, -2.0557036231, -1.5427121858\H, 3.2478209198, 1.58861752  
 08, -1.4545158637\C, 1.7150813561, 2.7074942651, -0.4979329651\C, 1.9335967  
 866, 2.3296784385, -2.9787884293\C, 2.6266904329, 3.2319056005, 0.421972455  
 \C, 2.2128633882, 4.1069233335, 1.4271625925\C, 0.8730510112, 4.4740511577,  
 1.5253651248\C, -0.0459735597, 3.9682131566, 0.6054764838\C, 0.3730745074,  
 3.0964570506, -0.3967052759\H, 3.6743581735, 2.9470337011, 0.3492565669\H,  
 2.9393040375, 4.5018570581, 2.1319750264\H, 0.5463019613, 5.1532086855, 2.3  
 072176574\H, -1.0908881901, 4.2602103334, 0.6672983206\H, -0.3548155761, 2.  
 7183535343, -1.112970196\H, 2.3269505821, 1.6571027622, -3.7484847257\H, 2.  
 4262607324, 3.3011872268, -3.0831585338\H, 0.8641100797, 2.4721766926, -3.1  
 709894218\H, -2.2527936007, -2.6715474265, 2.0468728929\H, -1.7096966886, -  
 2.92314295, 0.0112867168\H, -2.8148474042, -3.0645362811, -2.4350747245\H,  
 -1.7667417208, -2.5503242313, -3.7621244283\H, -2.6403674685, -1.341244443  
 7, -2.8041711894\H, -0.7649241548, -4.392316862, -1.6526317642\H, 0.7576475  
 73, -3.5621842663, -1.2655127021\H, 0.2223526887, -3.7071478495, -2.9506012  
 422\C, -3.7673791139, -1.3427237634, -0.2356850293\C, -4.8038230622, -0.414  
 7093547, -0.1575284683\C, -4.5396756347, 0.9553264176, -0.0535230413\C, -3.  
 1970807253, 1.3535532125, -0.0063859378\C, -2.1615200368, 0.4236392736, -0.  
 0752647791\H, -4.0054277773, -2.4025513523, -0.3119839278\H, -5.8357685895  
 , -0.7587818699, -0.1730846325\B, -5.8457565906, 2.4507169122, 1.6055535593  
 \H, -2.9584968676, 2.412085246, 0.09519208\H, -1.1306032312, 0.7516158856, 0.  
 0181556161\O, -6.9020918785, 3.2678374179, 1.8906278714\O, -5.0036091083,  
 2.1004774193, 2.6247252539\H, -6.9262398993, 3.5098083324, 2.828031266\H, -  
 4.2878091496, 1.5136774585, 2.3354468518\C, -5.6475246756, 1.9637963476, 0.  
 1045755608\H, -6.5995361701, 1.5599348724, -0.260242057\H, -5.448458914, 2.  
 8521146936, -0.5105230075\\Version=EM64L-G09RevC.01\\State=1-A\\HF=-1511.  
 3290072\\RMSD=6.403e-09\\RMSF=1.597e-06\\Dipole=0.6720563, -0.2730819, 0.09  
 97213\\Quadrupole=-0.3808118, -1.0040017, 1.3848135, 4.8951387, 0.0373383, 4  
 .2927404\\PG=C01 [X(C31H42B1N1O3)]\\@

**23-** (core)

1\\1\\GINC-R90\\FOpt\\UM062X\\Gen\\C9H14B1N1O4(1-,2)\\ROOT\\16-Aug-2014\\0\\#M0  
 62X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=80530  
 6368\\sbtnc\_rcore.freq\\-1,2\N, -2.8956090606, -0.139161316, -0.277299821  
 \O, -3.4242536413, -0.1184972527, -1.4388561231\C, -2.8585452267, -1.413044

5668, 0.4254038389\c, -1.8815616684, 0.8736255112, 0.0639898374\c, -0.48008  
 39522, 0.3173814488, 0.0392705729\h, -2.1146742876, 1.2580457876, 1.0656639  
 044\c, 0.1110652384, -0.0705504238, -1.1668723979\c, 1.3786310635, -0.64579  
 40159, -1.1814902762\c, 2.1116737587, -0.8620204281, 0.0015207658\c, 1.5087  
 956162, -0.4497314727, 1.204125621\c, 0.2392937828, 0.1180064285, 1.2220295  
 205\h, -0.4359157432, 0.0720602174, -2.0984379053\h, 1.8306945523, -0.93183  
 9168, -2.1288259885\B, 4.6394458578, -0.1773503694, 0.0199661938\h, 2.07614  
 36268, -0.5556536645, 2.1249455168\h, -0.2004327745, 0.4248201678, 2.171731  
 8629\o, 5.9976225234, -0.7418596138, -0.0384373386\o, 4.4198533277, 0.54213  
 74625, 1.2875892609\h, 6.3558300946, -0.4926073203, -0.8995828775\h, 5.2416  
 440936, 1.0164724384, 1.4703326319\c, 3.492670717, -1.4017013362, -0.022490  
 334\h, 3.6632636525, -1.9905310048, -0.9323874381\h, 3.6780408243, -2.04070  
 31167, 0.8500169697\o, 4.5017037067, 0.7126326755, -1.1625407298\h, 3.73376  
 03727, 1.2800466864, -1.0182029264\h, -3.8229654438, -1.9014643886, 0.27837  
 21477\h, -2.6746787652, -1.2352030985, 1.4885641968\h, -2.0520248526, -2.04  
 2762104, 0.0304229857\h, -2.0323373928, 1.6722858368, -0.6662916708\\Version=EM64L-G09RevC.01\\State=2-A\\HF=-731.7122698\\S2=0.755446\\S2-1=0.\\S2A=0.750018\\RMSD=3.118e-09\\RMSF=5.232e-06\\Dipole=-3.6646814, 0.0529729, 0.6973824\\Quadrupole=-34.4656418, 18.5592454, 15.9063964, 3.0493527, -11.9897295, 1.2603587\\PG=C01 [X(C9H14B1N1O4)]\\@

23-

1\\1\\GINC-R114\\FOpt\\UM062X\\Gen\\C15H26B1N1O4(1-,2)\\ROOT\\17-Aug-2014\\0\\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=134  
 2177280\\sbtnc\_r.freq\\-1,2\\N, -2.5619908579, -0.1176075211, -0.424970951  
 5\\o, -2.7272625001, -0.0592020046, -1.6890391969\\c, -4.3965810794, -1.68718  
 97634, -0.2136251214\\c, -1.6679318715, 2.1837935364, -0.4913956739\\c, -2.95  
 78967249, -1.3993988046, 0.2260754039\\c, -1.5663233536, 0.8034501556, 0.179  
 4969299\\c, -2.0253980589, -2.5233001466, -0.2470812636\\c, -0.1771787858, 0.  
 2003100956, 0.1410283523\\c, -2.9030130406, -1.2679848187, 1.747616153\\h, -1  
 .8791993565, -1.130762066, 2.1070600441\\h, -3.2915034143, -2.1910918058, 2.  
 1908665937\\h, -2.399091998, -3.4876196004, 0.1174512205\\h, -1.005974885, -2  
 .3770188356, 0.1213819763\\h, -1.9996804139, -2.5445061453, -1.3407815006\\h  
 , -5.0621549188, -0.8742016185, 0.0985715514\\c, -0.6695411167, 3.1439602934  
 , 0.1572739909\\h, -4.4521485414, -1.7817325086, -1.300081061\\c, -3.09086257  
 88, 2.7370721865, -0.3934894801\\h, -4.7412112966, -2.61979672, 0.2459394198  
 \\h, -1.4077065072, 2.0580091842, -1.5486371339\\h, -3.5242561417, -0.4353079  
 477, 2.0981310111\\h, -1.8596451105, 0.9331303117, 1.2289134911\\h, -0.880315  
 2742, 3.2576235788, 1.2295463165\\h, -0.7419498792, 4.1351990944, -0.3041718  
 817\\h, 0.3591850802, 2.7880805637, 0.0551653143\\h, -3.3962012296, 2.8207040  
 523, 0.6591037001\\h, -3.8060478734, 2.0934744825, -0.9122811345\\h, -3.14503  
 87546, 3.7391411652, -0.8343834918\\c, 0.4081864095, -0.1876120191, -1.06754  
 99247\\c, 1.6789165946, -0.7573329156, -1.087045979\\c, 2.4226661248, -0.9643  
 921377, 0.0905419012\\c, 1.8273268921, -0.546263882, 1.2948021258\\c, 0.55547  
 84398, 0.0170063864, 1.3180801239\\h, -0.1503812317, -0.0653485115, -1.99464  
 12354\\h, 2.1224445062, -1.0510531948, -2.036212789\\b, 4.9485413888, -0.2752  
 380607, 0.0813731977\\h, 2.4018092471, -0.6435265724, 2.21219081\\h, 0.124793  
 0581, 0.333831971, 2.269233757\\o, 6.3080053936, -0.8379952933, 0.0341875731  
 \\o, 4.7265214952, 0.4680233546, 1.3351286117\\h, 6.6689052529, -0.597334028,  
 -0.8282816624\\h, 5.5501940956, 0.9402404207, 1.5147666107\\c, 3.8047462167,  
 -1.5020479393, 0.0604162004\\h, 3.968813915, -2.099571633, -0.8450502545\\h,  
 3.9974683846, -2.1327563822, 0.9373912947\\o, 4.8103050699, 0.5927898062, -1  
 .1175891477\\h, 4.0431132303, 1.1635432372, -0.9830237914\\Version=EM64L-G  
 09RevC.01\\State=2-A\\HF=-967.4899919\\S2=0.75482\\S2-1=0.\\S2A=0.750015\\RM  
 SD=2.182e-09\\RMSF=4.019e-06\\Dipole=-6.0804307, 0.3917959, 0.6048896\\Quad  
 rupole=-46.054654, 23.8710246, 22.1836294, 7.2992473, -9.0027603, 1.0919019  
 \\PG=C01 [X(C15H26B1N1O4)]\\@

23^-P (core)

1\\1\\GINC-R306\\FOpt\\RM062X\\Gen\\C13H21B1N1O4(1-)\\ROOT\\22-Aug-2014\\0\\#M0  
 62X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=10737  
 41824\\pssbntc\_core.freq\\-1,1\\N, 0.5121077594, 0.9663331713, -0.36368942  
 35\\o, 1.7227314549, 1.4762595297, 0.202479895\\c, 2.7065237563, 0.4576525024  
 , 0.1983333236\\c, 2.3662368475, -0.6479339456, 1.1967614634\\c, 4.036227354,  
 1.0850117912, 0.5122122392\\c, 0.3119817539, 1.6992492237, -1.6063581269\\c,  
 -0.5442828168, 1.2534849928, 0.6199717882\\c, -1.8876228816, 0.7729381549, 0  
 .1381632794\\h, 1.4005644033, -1.0906056879, 0.9385283696\\h, 2.314735703, -0  
 .2304283294, 2.2078030005\\h, 2.7499645291, 0.0196356335, -0.8125748671\\c, 4  
 .2397653889, 2.3781589479, 0.7572165342\\h, 3.4181581885, 3.0866440534, 0.73  
 08912261\\h, -0.5747773559, 2.3367554621, 0.8285647827\\c, -2.9066296049, 1.6  
 717991468, -0.1933115563\\c, -4.136104692, 1.224550544, -0.6670694842\\c, -4.  
 4009397576, -0.1451829165, -0.8474601425\\c, -3.3707663772, -1.0389236759,-

0.4988064511\c, -2.1431686239, -0.5924548839, -0.0171815594\h, -2.73313347  
 47, 2.7407572318, -0.0690620919\h, -4.9329410198, 1.9329146952, -0.87815689  
 48\B, -6.8233049756, -0.6963458426, -0.0117906472\h, -3.5549160838, -2.1062  
 608326, -0.6033012134\h, -1.3631646332, -1.3106526655, 0.2344549787\o, -6.9  
 597657891, 0.6839945954, 0.4854410524\o, -8.1210867659, -1.2239102041, -0.4  
 664166183\h, -7.7831285244, 0.7056198724, 0.9908029092\h, -8.207805527, -2.  
 1005999636, -0.0715596314\c, -5.7357130138, -0.6245471681, -1.2857701939\h  
 , -5.6609911677, -1.6291842787, -1.7210957169\h, -6.1656069628, 0.050944525  
 4, -2.0361784437\o, -6.3385912137, -1.6289678311, 1.0408469809\h, -5.612444  
 0859, -1.1960756956, 1.5078269953\h, 3.1287279435, -1.4346833186, 1.1790022  
 593\h, 4.870790717, 0.3838796918, 0.5475325285\h, -0.602716648, 1.331982904  
 4, -2.0765012525\h, 1.1626333074, 1.5088346727, -2.2663005995\h, 0.22391393  
 38, 2.783891068, -1.4310919923\h, -0.2452718889, 0.7450854522, 1.5435522269  
 \h, 5.231780844, 2.7547293768, 0.9900310733\Version=EM64L-G09RevC.01\State=1-A\HF=-888.2716889\RMSD=4.137e-09\RMSF=4.176e-06\Dipole=6.8635953,  
 1.0719597, 0.1766225\Quadrupole=-49.7885865, 24.3907548, 25.3978317, -18.6  
 102802, -4.0446293, -0.2314518\PG=C01 [X(C13H21B1N1O4)]\@\@

23<sup>-</sup>P

1\1\GINC-R281\FOpt\RM062X\Gen\C31H43B1N1O4(1-)\ROOT\24-Aug-2014\0\#\#M0  
 62X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=24159  
 19104\pssbtnc.freq\`-1,1\N,-0.1241141685,-1.8799039855,0.3646527414\o  
 ,-1.0925626019,-1.46105096,1.3090434318\c,-1.7238520451,-0.2344306445,  
 0.9030386578\c,-1.080091291,0.9462512398,1.6391196955\c,-3.1976631002,  
 -0.3607513579,1.2176664241\c,-0.7254788503,-4.2961479285,0.7286764852\c,  
 1.3678950631,-1.4508218983,2.3858537199\c,-0.5835865321,-3.136345162  
 9,-0.2677845717\c,1.2689186267,-1.8787900369,0.8980732665\c,-1.9447889  
 585,-2.8674199183,-0.9197406629\c,2.1315666463,-1.0598912176,-0.057802  
 8177\c,0.413965902,-3.4920955018,-1.3777001878\h,0.5543505448,-2.64112  
 86686,-2.0512752441\h,0.0225649225,-4.3406810477,-1.9500985028\h,-2.27  
 12443736,-3.7553405572,-1.4728717025\h,-1.8704951392,-2.0306780841,-1.  
 6236238031\h,-2.706949904,-2.632036736,-0.1712617291\h,-1.0836982918,-  
 5.1950269563,0.2129473916\c,2.813183447,-1.1910954783,2.818603045\h,0.  
 2309708494,-4.5392950698,1.2037867339\c,0.7560574554,-2.5113582354,3.3  
 071685924\h,-1.4470038301,-4.0373252852,1.5107613321\h,0.813183115,-0.  
 5192852808,2.5155394266\h,-0.0133245893,0.9686532814,1.3835105272\c,-1  
 .6934340632,2.323405265,1.3455398694\h,-1.1511326995,0.7414178698,2.71  
 74479762\h,-1.5908605385,-0.1185865272,-0.1787980919\c,-4.1615736615,0  
 .0223426794,0.2832800245\c,-5.5203471571,-0.0657832217,0.5864656408\c,  
 -5.9282694818,-0.5493216881,1.8283402801\c,-4.9705852584,-0.9449093873  
 ,2.7633790553\c,-3.614209712,-0.8486883823,2.4603058099\h,-3.839966382  
 2,0.3892621422,-0.6895154915\h,-6.2592641854,0.2361695283,-0.150967955  
 5\h,-6.9860810166,-0.622854239,2.0655158934\h,-5.2823105942,-1.3306154  
 512,3.7304144884\h,-2.8654519864,-1.1660604048,3.1824324987\h,-2.78270  
 38088,2.2540656049,1.4728374361\c,-1.4226447828,2.7997645203,-0.072028  
 4701\c,-1.1688398748,3.3492377779,2.3607295049\c,-2.4791000054,3.12247  
 71813,-0.9289324993\c,-2.2352885467,3.6175000291,-2.2112099476\c,-0.92  
 5856291,3.8066486246,-2.6493342558\c,0.1428244487,3.4924716649,-1.8072  
 324862\c,-0.1124930059,2.9866872653,-0.5330980023\h,-3.5032938597,2.99  
 16858794,-0.5822250434\h,-3.0707595265,3.8605676434,-2.8634153254\h,-0  
 .7337344213,4.1974735445,-3.6449085838\h,1.1777607538,3.6336168067,-2.  
 1216933401\h,0.7358465055,2.7341784586,0.1013594428\h,-1.4423680505,3.  
 0584167532,3.3814575224\h,-1.5818605372,4.3425718262,2.1579188098\h,-0  
 .076847416,3.4228990286,2.3093303316\h,1.3964104289,-3.7745656613,-0.9  
 88941427\h,1.6543143041,-2.9119157096,0.8888304161\h,3.4321654975,-2.0  
 887764918,2.6902295422\h,2.8305208749,-0.9281077669,3.8829173468\h,3.2  
 777390829,-0.3800426246,2.2536349944\h,1.3176237679,-3.452559758,3.226  
 9113118\h,-0.2898844669,-2.7104411024,3.0660069976\h,0.8127827173,-2.1  
 838715027,4.3524746395\c,3.4952086876,-1.3262185348,-0.2159329069\c,4.  
 2961426847,-0.5437498526,-1.0481109773\c,3.7672672474,0.5234536218,-1.  
 7902330162\c,2.3874341908,0.7452160919,-1.6644440735\c,1.5926430818,-0  
 .0159717038,-0.8168376044\h,3.9464581015,-2.1558056728,0.329310424\h,5  
 .3596808847,-0.7601998582,-1.1266055788\B,4.7877333879,2.930871686,-1.  
 9388424027\h,1.9444373992,1.5524346975,-2.2389114817\h,0.5266822216,0.  
 1858400064,-0.7688698666\o,5.3849745848,2.8087676024,-0.5896756702\o,5  
 .6712388038,3.7450422423,-2.8060096463\h,6.217293719,3.2955218782,-0.6  
 300721776\h,5.1768314208,4.550790082,-3.0008362454\c,4.5936083446,1.43  
 17358593,-2.6320506079\h,4.1072533882,1.5895260985,-3.605206941\h,5.58  
 5292744,0.9993411921,-2.8197121695\o,3.458743502,3.6027486393,-1.80930  
 9604\h,3.4097036583,3.8619312409,-0.8792476157\Version=EM64L-G09RevC.  
 01\State=1-A\HF=-1587.192563\RMSD=3.702e-09\RMSF=3.376e-06\Dipole=-6.3

762414,-2.8191577,2.7939994\Quadrupole=-29.2650597,9.8902422,19.374817  
5,-29.3563142,28.602832,13.9108078\PG=C01 [X(C31H43B1N1O4)]\\@