SUPPORTING INFORMATION

Catalytic Enantioselective [3+2] Cycloadditions of Diazoketone-derived Aryl-substituted Carbonyl Ylides

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(a) MeOH, $(\text{MeO})_3\text{CH}$, H_2SO_4 , reflux, 18 h; (b) $\text{Me}(\text{MeO})\text{NH}\cdot\text{HCl}$, $i\text{-PrMgCl}$, THF, -10°C , 2.5 h; (c) BnMgCl , THF, 0°C , 2 h; (d) $4\text{-(NHAc)C}_6\text{H}_4\text{SO}_2\text{N}_3$, DBU, MeCN, 0°C , 6-16 h, then 10% citric acid;¹⁶ (e) MeMgBr , THF, 0°C , 1.5 h; (f) $t\text{-BuOK}$, $4\text{-(NO}_2\text{)C}_6\text{H}_4\text{CHO}$, NH_3 , -70°C , 8 h;²² (g) $4\text{-(NHAc)C}_6\text{H}_4\text{SO}_2\text{N}_3$, Et_3N , MeCN, 0°C , 2 h, then 10% citric acid.

Scheme S1. Synthesis of diazodione substrates **8**, **9**, **12** and **13**.

Experimental Section

General Methods

All reactions requiring anhydrous conditions were conducted in flame or oven-dried apparatus under an atmosphere of argon. Syringes and needles for the transfer of reagents were oven-dried and allowed to cool in a desiccator over self-indicating silica gel or P_2O_5 prior to use. All solvents were distilled before use. Ethers were distilled from sodium / benzophenone ketyl; (halogenated) hydrocarbons and MeCN from CaH_2 . MeOH was distilled from magnesium. 'Petrol' refers to the fraction of light petroleum ether boiling between 40-60 °C. $Rh_2(OAc)_4$ and $Rh_2(S-DOSP)_4$ were purchased from Aldrich Chemical Company. Hashimoto's procedure was followed for the preparation of $Rh_2(S-BPTV)_4$.^{12a} $Rh_2(R-BNP)_4$ was prepared according to Pirrung's method⁸ and $Rh_2(R-DDBNP)_4$ as we reported.^{9b} Reactions were monitored by TLC using commercially available aluminium or glass backed plates pre-coated with silica (0.25 mm, Merck 60 F₂₅₄) which were developed using standard visualising techniques: UV fluorescence (254 nm) and / or potassium permanganate or vanillin solution, Δ . Flash chromatography was performed on either Kieselgel 60 (40-63 μ m) or Florisil[®] (200 mesh).

Synthesis of Diazodione 8

Methyl 4,4-dimethoxynon-8-enoate 4-Oxo-8-nonenoic acid^{9b} (15.5 g, 91.2 mmol), sulfuric acid (10 drops, catalytic) and trimethyl orthoformate (300 cm³) in MeOH (400 cm³) were heated at reflux temperature for 18 h. The reaction mixture was allowed to cool then diluted with Et₂O and washed with a 1:1 mixture of NaOH solution (5% aq.) and brine, water and brine. The organic layer was dried (MgSO₄) and evaporated to give the title compound as a yellow oil (21.0 g, quant.): R_f = 0.35 (1:1 petrol:Et₂O); IR (neat) 2953, 2831, 1742, 1642, 1437, 1315, 1172, 1054

cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 5.77 (1H, ddt, J = 17, 10, 7 Hz), 5.02–4.93 (2H, m), 3.66 (3H, s), 3.13 (6H, s), 2.28–2.23 (2H, m), 2.03 (2H, q, J = 7 Hz), 1.94–1.89 (2H, m), 1.54–1.50 (2H, m), 1.38–1.31 (2H, m); ¹³C NMR (100 MHz, CDCl₃) δ 173.7, 138.2, 115.0, 102.4, 51.6, 47.8, 33.7, 31.8, 28.9, 27.6, 22.8; MS (ES) m/z 253 (M + Na⁺, 100), 199 (79), 167 (18); HRMS (ES) calcd for C₁₂H₂₂O₄Na 253.1416, found 253.1417 (M + Na⁺).

***N*-Methoxy-*N*-methyl-4,4-dimethoxynon-8-enamide** Methyl 4,4-dimethoxynon-8-enoate (3.84 g, 16.7 mmol) and *N,O*-dimethylhydroxylamine hydrochloride (2.44 g, 25.0 mmol) in THF (80 cm³) were cooled to –20 °C. Isopropylmagnesium chloride (2.0 M in THF, 25 cm³, 50.0 mmol) was added slowly and the resulting mixture stirred for 2 h allowing to warm to –10 °C. NH₄Cl Solution (20% aq.) was added and the mixture extracted with Et₂O. The organic layers were combined, washed with water, dried (Na₂SO₄) and evaporated to give the title compound as a yellow oil (3.97 g, 92 %): R_f = 0.10 (1:1 petrol:Et₂O); IR (neat) 2951, 2830, 1667, 1461, 1180, 1051 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 5.79 (1H, ddt, J = 17, 10, 7 Hz), 5.06–4.93 (2H, m), 3.69 (3H, s), 3.18 (3H, s), 3.17 (6H, s), 2.42–2.38 (2H, m), 2.06 (2H, q, J = 7 Hz), 1.96–1.91 (2H, m), 1.60–1.56 (2H, m), 1.43–1.35 (2H, m); ¹³C NMR (100 MHz, CDCl₃) δ 173.9, 138.3, 115.0, 102.8, 61.2, 47.8, 33.8, 32.2, 31.9, 27.2, 26.8, 22.8; MS (APCI) m/z 282 (M + Na⁺, 9), 228 (M – OMe, 100), 139 (17), 125 (17); HRMS (ES) calcd for C₁₃H₂₅NO₄Na 282.1681, found 282.1683 (M + Na⁺).

5,5-Dimethoxy-1-phenyldec-9-en-2-one *N*-Methoxy-*N*-methyl-4,4-dimethoxynon-8-enamide (2.20 g, 8.49 mmol) in THF (40 cm³) was cooled to 0 °C. Benzylmagnesium chloride (1.0 M in Et₂O, 17.0 cm³, 17.0 mmol) was added slowly and the resulting mixture stirred for 2 h. NH₄Cl Solution (saturated aq.) was added and the mixture extracted with Et₂O. The organic layers were combined, washed with brine, dried (MgSO₄), evaporated and the residue purified by column

chromatography (Florisil[®], 12:1 petrol:EtOAc) to give the title compound as a colorless oil (1.94 g, 79%): R_f = 0.30 (3:1 petrol:Et₂O); IR (neat) 2946, 2832, 1708, 1640, 1497, 1454, 1409, 1360 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.38–7.20 (5H, m), 5.74 (1H, ddt, J = 17, 10, 7 Hz), 5.02–4.95 (2H, m), 3.71 (2H, s), 3.10 (6H, s), 2.44–2.40 (2H, m), 2.01 (2H, q, J = 7 Hz), 1.87–1.84 (2H, m), 1.50–1.45 (2H, m), 1.32–1.26 (2H, m); ¹³C NMR (100 MHz, CDCl₃) δ 207.5, 138.2, 134.1, 129.4, 128.7, 127.0, 115.1, 102.6, 50.2, 47.8, 36.5, 33.7, 32.0, 26.4, 22.8; MS (APCI) m/z 313 (M + Na⁺, 6), 259 (M – OMe, 100), 245 (25), 175 (94), 147 (22).

1-Diazo-1-phenyldec-9-ene-2,5-dione (8) 5,5-Dimethoxy-1-phenyldec-9-en-2-one (3.01 g, 10.38 mmol) and 4-acetamidobenzenesulfonyl azide (2.99 g, 12.44 mmol) in MeCN (60 cm³) were cooled to 0 °C before dropwise addition of DBU (1.86 cm³, 12.44 mmol). The mixture was stirred for 6 h before the solvent was evaporated and replaced with THF (60 cm³). Citric acid solution (10% aq., 100 cm³) was added and the mixture stirred vigorously for 0.5 h before extraction with Et₂O. The organic layers were combined, washed with NaHCO₃ (saturated aq.), water, dried (MgSO₄), evaporated and the residue purified by column chromatography (Florisil[®], 10:1 petrol:EtOAc) to give **8** as an orange-yellow oil which solidified on standing (1.54 g, 55%): mp 34–36 °C (petrol:Et₂O); R_f = 0.50 (1:1 petrol:Et₂O); IR (neat) 2932, 2074, 1714, 1648, 1498, 1369, 1210 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.51–7.49 (2H, m), 7.42–7.38 (2H, m), 7.27–7.23 (1H, m), 5.77 (1H, ddt, J = 17, 10, 7 Hz), 5.05–4.97 (2H, m), 2.89–2.80 (4H, m), 2.51 (2H, t, J = 7.5 Hz), 2.07 (2H, q, J = 7 Hz), 1.71 (2H, quin., J = 7.5 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 209.2, 191.8, 137.9, 129.0, 127.0, 126.0, 125.0, 115.2, 72.4, 41.9, 36.4, 33.0, 32.5, 22.7. Anal. Calcd for C₁₆H₁₈N₂O₂: C, 71.1; H, 6.7; N, 10.4. Found: C, 71.4; H, 6.9; N, 9.9.

Synthesis of Diazodione 9

5,5-Dimethoxydec-9-en-2-one *N*-Methoxy-*N*-methyl-4,4-dimethoxynon-8-enamide (12.5 g, 48.3 mmol) in THF (200 cm³) was cooled to 0 °C. Methylmagnesium bromide (3.0 M in Et₂O, 32.2 cm³, 96.5 mmol) was added slowly and the resulting mixture stirred for 2 h. NH₄Cl Solution (saturated aq.) was added and the mixture extracted with Et₂O. The organic layers were combined, washed with water, dried (MgSO₄) and evaporated to give the title compound as a yellow oil (9.56 g, 92%): *R*_f = 0.55 (1:1 petrol:Et₂O); IR (neat) 2952, 2830, 1719, 1460, 1353 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 5.79 (1H, ddt, *J* = 17, 10, 7 Hz), 5.05–4.96 (2H, m), 3.14 (6H, s), 2.43–2.39 (2H, m), 2.16 (3H, s), 2.05 (2H, q, *J* = 7 Hz), 1.90–1.86 (2H, m), 1.55–1.51 (2H, m), 1.39–1.31 (2H, m); ¹³C NMR (100 MHz, CDCl₃) δ 207.7, 138.0, 114.9, 102.4, 47.6, 38.1, 33.6, 31.9, 29.8, 26.1, 22.7; MS (APCI) *m/z* 183 (*M* – OMe, 100), 141 (39), 109 (36); HRMS (ES) calcd for C₁₂H₂₆NO₃ 232.1913, found 232.1913 (*M* + NH₄⁺).

5,5-Dimethoxy-1-(4-nitrophenyl)dec-9-en-2-one Potassium *tert*-butoxide (6.29 g, 56.1 mmol) was added to ammonia (200 cm³) at –70 °C. 4-Nitrobenzaldehyde (2.12 g, 14.0 mmol) was added and the mixture stirred for 5 min before the dropwise addition of neat 5,5-dimethoxydec-9-en-2-one (9.00 g, 42.1 mmol). The mixture was stirred at –70 °C for 10 h. Excess NH₄Cl (s) and Et₂O were added and the ammonia allowed to evaporate overnight. Water was added and the Et₂O layer separated. The aqueous layer was further extracted with Et₂O, the organic layers combined, dried (Na₂SO₄), evaporated and the residue purified by column chromatography (Florisil[®], 10:1 cyclohexane:EtOAc) to give the title compound as a yellow oil (1.07 g, 23 %): *R*_f = 0.35 (1:1 petrol:Et₂O); IR (neat) 2950, 1718, 1606, 1521, 1347 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.17 (2H, d, *J* = 9 Hz), 7.35 (2H, d, *J* = 9 Hz), 5.74 (1H, ddt, *J* = 17, 10, 7 Hz), 5.02–4.93 (2H, m), 3.85 (2H, s), 3.10 (6H, s), 2.51–2.47 (2H, m), 2.02 (2H, q, *J* = 7 Hz), 1.91–1.87 (2H, m), 1.54–1.49 (2H, m), 1.36–1.27 (2H, m); ¹³C NMR (100 MHz, CDCl₃) δ

205.5, 147.0, 141.5, 138.1, 130.4, 123.7, 115.1, 102.5, 49.2, 47.8, 37.3, 34.0, 32.1, 26.3, 23.2; MS (ES) m/z 335 (M^+ , 20), 334 ($M + H^+$, 100), 288 (48); HRMS (ES) calcd for $C_{18}H_{24}NO_5$ 334.1654, found 334.1658 ($M - H^+$).

1-Diazo-1-(4-nitrophenyl)dec-9-ene-2,5-dione (9) 5,5-Dimethoxy-1-(4-nitrophenyl)dec-9-en-2-one (1.03 g, 3.07 mmol) and 4-acetamidobenzenesulfonyl azide (886 mg, 3.69 mmol) in MeCN (15 cm³) were cooled to 0 °C before dropwise addition of Et₃N (0.51 cm³, 3.69 mmol). After 2.5 h citric acid solution (10% aq.) was added and the mixture stirred vigorously for 1.5 h before extraction with Et₂O. The organic layers were combined, washed with water, NaHCO₃ (saturated aq.), brine, dried (MgSO₄), evaporated and the residue purified by column chromatography (SiO₂, 8:1 cyclohexane:EtOAc) to give **9** as a bright yellow solid (453 mg, 47%); R_f = 0.20 (1:1 petrol:Et₂O); IR (KBr disc) 2917, 2089, 1708, 1647, 1592, 1512, 1343 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.21 (2H, d, J = 9 Hz), 7.72 (2H, d, J = 9 Hz), 5.76 (1H, ddt, J = 17, 10, 7 Hz), 5.03–4.96 (2H, m), 2.93–2.84 (4H, m), 2.51 (2H, t, J = 7.5 Hz), 2.06 (2H, q, J = 7 Hz), 1.70 (2H, quin., J = 7.5 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 209.0, 190.1, 145.5, 137.8, 133.5, 124.4, 124.1, 115.3, 73.2, 41.8, 36.3, 33.0, 32.7, 22.7; MS (FAB) m/z 338 ($M + Na^+$, 9), 316 ($M + H^+$, 66), 291 (26), 166 (58), 152 (100); HRMS (ES) calcd for $C_{16}H_{18}N_3O_4$ 316.1297, found 316.1297 ($M + H^+$). Anal. Calcd for $C_{16}H_{17}N_3O_4$: C, 60.9; H, 5.4; N, 13.3. Found: C, 61.0; H, 5.4; N, 13.1.

Cycloaddition Reactions of **8** and **9**

7-Phenyl-11-oxatricyclo[5.3.1.0^{1,5}]undecan-8-one (10) General Procedure: A Rh(II) catalyst (0.5–1 mol%) was added to 1-diazo-1-phenyldec-9-ene-2,5-dione (**8**) (~ 70 mg, ~ 0.26 mmol) in the desired solvent (3 cm³) and the mixture stirred until no starting material remained by TLC. The solvent was evaporated and the residue purified by column chromatography (SiO₂, 5:1 → 1:1 petrol:CH₂Cl₂) to give **10** as a colourless oil which remained a solid after freezing: mp 52–53 °C

(petrol); $R_f = 0.45$ (3:1 petrol:Et₂O); IR (KBr disc) 2941, 2867, 1716, 1448, 1038 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.46–7.44 (2H, m), 7.37–7.27 (3H, m), 2.84–2.71 (2H, m), 2.57–2.48 (3H, m), 2.17–2.12 (1H, m), 1.95–1.82 (3H, m), 1.80–1.65 (2H, m), 1.61–1.49 (2H, m); ¹³C NMR (100 MHz, CDCl₃) δ 211.3, 138.4, 127.9, 127.5, 126.0, 92.2, 91.9, 46.8, 46.2, 37.6, 34.9, 33.9, 33.2, 24.7; MS (APCI) m/z 243 (M + H⁺, 55), 225 (100), 197 (33); HRMS (ES) calcd for C₁₆H₂₂NO₂ 260.1651, found 260.1647 (M + NH₄⁺). Anal. Calcd for C₁₆H₁₈O₂: C, 79.3; H, 7.5. Found: C, 79.3; H, 7.65.

7-(4-Nitrophenyl)-11-oxatricyclo[5.3.1.0^{1,5}]undecan-8-one (11) General procedure as for **10** above, replacing **8** with 1-diazo-1-(4-nitrophenyl)dec-9-ene-2,5-dione (**9**) and purification by column chromatography (SiO₂, 6:1 cyclohexane:Et₂O) to give **11** as yellow crystals: mp 101 °C (petrol:Et₂O); $R_f = 0.50$ (1:1 petrol:Et₂O); IR (KBr disc) 2954, 2866, 1713, 1603, 1519, 1352 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.18 (2H, d, $J = 9$ Hz), 7.60 (2H, d, $J = 9$ Hz), 2.83 (1H, dd, $J = 13, 9$ Hz), 2.73–2.65 (1H, m), 2.63–2.47 (3H, m), 2.17–2.12 (1H, m), 2.00–1.81 (3H, m), 1.75–1.67 (2H, m), 1.62–1.56 (1H, m), 1.52–1.48 (1H, m); ¹³C NMR (100 MHz, CDCl₃) δ 208.5, 147.1, 145.6, 127.0, 122.9, 93.0, 91.1, 46.5, 46.5, 37.3, 34.7, 34.0, 33.3, 24.8 (CH₂); MS (EI) m/z 288 (M + H⁺, 100), 270 (35). Anal. Calcd for C₁₆H₁₇NO₄: C, 66.9; H, 6.0; N, 4.9. Found: C, 66.6; H, 6.1; N, 4.75.

Synthesis of Diazodione 12

Methyl 4,4-dimethoxypentanoate Levulinic acid (10.2 g, 87.8 mmol), 4-toluenesulfonic acid (60 mg, catalytic) and trimethylorthoformate (80 cm³) in MeOH (120 cm³) were heated at reflux temperature for 18 h. The reaction mixture was allowed to cool then diluted with Et₂O and washed with a 1:1 mixture of NaOH solution (5% aq.) and brine, water and brine. The organic layer was dried (MgSO₄) and evaporated to give the title compound as a yellow oil (15.0 g, 97%): $R_f = 0.40$ (1:1 petrol:Et₂O); IR (neat) 2953, 2832, 1741, 1437, 1380, 1172, 1053 cm⁻¹; ¹H NMR

(400 MHz, CDCl₃) δ 3.65 (3H, s), 3.14 (6H, s), 2.32 (2H, dd, $J = 8, 8$ Hz), 1.93 (2H, dd, $J = 8, 8$ Hz), 1.21 (3H, s); ¹³C NMR (100 MHz, CDCl₃) δ 173.7, 100.8, 51.6, 48.1, 31.4, 29.3, 20.7; MS (APCI) m/z 145 (M – OMe, 47), 113 (100); HRMS (ES) calcd for C₇H₁₃O₃ 145.0865, found 145.0868 (M – OMe).

***N*-Methoxy-*N*-methyl-4,4-dimethoxypentanamide** Methyl 4,4-dimethoxypentanoate (17.6 g, 100 mmol) and *N,O*-dimethylhydroxylamine hydrochloride (14.6 g, 150 mmol) in THF (200 cm³) were cooled to –10 °C. Isopropylmagnesium chloride (2.0 M in THF, 150 cm³, 300 mmol) was added slowly and the resulting mixture stirred for 2.5 h maintaining the low temperature. NH₄Cl Solution (20% aq.) was added and the mixture extracted with Et₂O. The organic layers were combined, washed with water, dried (Na₂SO₄) and evaporated to give the title compound as a yellow oil (17.0 g, 83 %): $R_f = 0.15$ (1:1 petrol:Et₂O); IR (neat) 2945, 2830, 1667, 1464, 1380, 1175, 1052 cm^{–1}; ¹H NMR (400 MHz, CDCl₃) δ 3.63 (3H, s), 3.11 (3H, s), 3.11 (6H, s), 2.38 (2H, dd, $J = 8, 8$ Hz), 1.89 (2H, dd, $J = 8, 8$ Hz), 1.20 (3H, s); ¹³C NMR (100 MHz, CDCl₃) δ 174.0, 101.0, 61.1, 48.0, 32.1, 30.9, 27.0, 20.7; MS (APCI) m/z 228 (M + Na⁺, 50), 174 (M – OMe, 100); HRMS (ES) calcd for C₈H₁₆NO₃ 174.1130, found 174.1128 (M – OMe).

5,5-Dimethoxy-1-phenylhexan-2-one *N*-Methoxy-*N*-methyl-4,4-dimethoxypentanamide (12.6 g, 61.5 mmol) in THF (250 cm³) was cooled to 0 °C. Benzylmagnesium chloride (2.0 M in THF, 61.5 cm³, 123 mmol) was added slowly and the resulting mixture stirred for 2 h. NH₄Cl Solution (saturated aq.) was added and the mixture extracted with Et₂O. The organic layers were combined, washed with brine, dried (MgSO₄), evaporated and the residue purified by column chromatography (Florisil[®], 20:1 cyclohexane:EtOAc) to give the title compound as a colourless oil (10.9 g, 75%): $R_f = 0.50$ (1:1 petrol:Et₂O); IR (neat) 2946, 2830, 1715, 1602, 1496, 1455, 1379m cm^{–1}; ¹H NMR (400 MHz, CDCl₃) δ 7.34–7.18 (5H, m), 3.69 (2H, s), 3.12 (6H, s), 2.50 (2H, dd, $J = 8, 8$ Hz), 1.89 (2H, dd, $J = 8, 8$ Hz), 1.18 (3H, s); ¹³C NMR (100 MHz, CDCl₃) δ

207.5, 134.2, 129.4, 128.7, 127.0, 101.1, 50.2, 48.2, 37.1, 30.2, 20.9; MS (CI, NH₃) *m/z* 205 (M – OMe, 100), 173 (21); HRMS (ES) calcd for C₁₄H₂₄NO₃ 254.1756, found 254.1754 (M + NH₄⁺).

1-Diazo-1-phenylhexane-2,5-dione (12) 5,5-Dimethoxy-1-phenylhexan-2-one (1.58 g, 6.69 mmol) and 4-acetamidobenzenesulfonyl azide (1.93 g, 8.03 mmol) in MeCN (25 cm³) were cooled to 0 °C before dropwise addition of DBU (1.20 cm³, 8.03 mmol). After 16 h citric acid solution (10% aq.) was added and the mixture stirred vigorously for 15 min before extraction with Et₂O. The organic layers were combined, washed with NaHCO₃ (saturated aq.), water, dried (MgSO₄), evaporated and the residue purified by column chromatography (Florisil[®], 1:1 petrol:Et₂O) to give **12** as an orange oil which remained solid after freezing (935 mg, 65%): mp 26–27 °C; *R*_f = 0.55 (1:1 petrol:Et₂O); IR (neat) 2076, 1717, 1647, 1497, 1363, 1211 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.51–7.48 (2H, m), 7.42–7.38 (2H, m), 7.27–7.23 (1H, m), 2.85 (4H, s), 2.23 (3H, s); ¹³C NMR (125 MHz, CDCl₃) δ 207.5, 191.6, 129.5, 127.5, 126.4, 125.9, 72.9, 37.7, 33.0, 30.4.

Synthesis of Diazodione 13

5,5-Dimethoxyhexan-2-one²³ *N*-Methoxy-*N*-methyl-4,4-dimethoxypentanamide (9.88 g, 48.1 mmol) in THF (150 cm³) was cooled to 0 °C. Methylmagnesium bromide (3.0 M in Et₂O, 32.0 cm³, 96.0 mmol) was added slowly and the resulting mixture stirred for 1.5 h. NH₄Cl Solution (saturated aq.) was added and the mixture extracted with Et₂O. The organic layers were combined, washed with water, dried (MgSO₄) and evaporated to give the title compound as a yellow oil (7.75 g, quant.): *R*_f = 0.30 (1:1 petrol:Et₂O); IR (neat) 2951, 2831, 1719, 1436, 1379 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 3.15 (6H, s), 2.47 (2H, dd, *J* = 8, 8 Hz), 2.14 (3H, s), 1.89 (2H, dd, *J* = 8, 8 Hz), 1.22 (3H, s); ¹³C NMR (100 MHz, CDCl₃) δ 208.0, 101.0, 48.1, 38.7, 30.0,

29.9, 20.9; MS (APCI) m/z 129 (M – OMe, 100), 115 (58), 111 (85); HRMS (ES) calcd for $C_7H_{13}O_2$ 129.0916, found 129.0914 (M – OMe).

5,5-Dimethoxy-1-(4-nitrophenyl)hexan-2-one Potassium *tert*-butoxide (1.50 g, 13.3 mmol) was added to ammonia (50 cm³) at – 70 °C. 4-Nitrobenzaldehyde (504 mg, 3.3 mmol) was added and the mixture stirred for 5 min before the dropwise addition of neat 5,5-dimethoxyhexan-2-one (1.60 g, 10.0 mmol). The mixture was stirred at – 70 °C for 8 h. Excess NH₄Cl (s) and Et₂O were added and the ammonia allowed to evaporate overnight. Water was added and the Et₂O layer separated. The aqueous was further extracted with Et₂O, the organic layers combined, dried (Na₂SO₄), evaporated and the residue purified by column chromatography (Florisil[®], 10:1 petrol:EtOAc) to give the title compound as a yellow oil (345 mg, 37 %): R_f = 0.25 (1:1 petrol:Et₂O); IR (neat) 2947, 2831, 1718, 1606, 1520, 1348 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.19 (2H, d, J = 9 Hz), 7.36 (2H, d, J = 9 Hz), 3.85 (2H, s), 3.12 (6H, s), 2.57 (2H, t, J = 8 Hz), 1.93 (2H, t, J = 8 Hz), 1.23 (3H, s); ¹³C NMR (100 MHz, CDCl₃) δ 205.5, 147.0, 141.5, 130.4, 123.7, 100.9, 49.2, 48.2, 37.9, 30.2, 20.9; MS (CI, NH₃) m/z 250 (M – OMe, 46), 220 (100), 205 (14), 188 (27), 167 (13), 106 (12); HRMS (ES) calcd for $C_{13}H_{16}NO_4$ 250.1079, found 250.1082 (M – OMe).

1-Diazo-1-(4-nitrophenyl)hexane-2,5-dione (13) 5,5-Dimethoxy-1-(4-nitrophenyl)hexan-2-one (300 mg, 1.07 mmol) and 4-acetamidobenzenesulfonyl azide (308 mg, 1.28 mmol) in MeCN (5 cm³) were cooled to 0 °C before dropwise addition of Et₃N (0.18 cm³, 1.28 mmol). After 2 h citric acid solution (10% aq.) was added and the mixture stirred vigorously for 0.5 h before extraction with Et₂O. The organic layers were combined, washed with NaHCO₃ (saturated aq.), water, dried (MgSO₄), evaporated and the residue purified by column chromatography (SiO₂, 4:1 petrol:EtOAc) to give **13** as a bright orange solid (179 mg, 64%): R_f = 0.20 (1:1 petrol:Et₂O); mp 117 °C (petrol:Et₂O); IR (KBr disc) 2086, 1714, 1648, 1594, 1511, 1342 cm⁻¹; ¹H NMR (400

MHz, CDCl₃) δ 8.19 (2H, d, J = 9 Hz), 7.70 (2H, d, J = 9 Hz), 2.89 (4H, s), 2.22 (3H, s); ¹³C NMR (100 MHz, CDCl₃) δ 206.0, 190.0, 145.6, 133.5, 124.5, 124.2, 73.2, 37.1, 32.7, 29.8; MS (EI) m/z 261 (M⁺, 6), 233 (50), 205 (100). Anal. Calcd for C₁₂H₁₁N₃O₄: C, 55.2; H, 4.2; N, 16.1. Found: C, 55.2; H, 4.2; N, 16.0.

Cycloaddition Reactions of **12** and **13**

General procedure for intermolecular cycloadditions: A Rh(II) catalyst (0.5–1 mol%) was added to diazodione **12** or **13** (~ 0.16 mmol) and the dipolarophile (~ 0.80 mmol, except DMAD ~ 0.35 mmol) in the desired solvent (3 cm³) and the mixture stirred until no starting material remained by TLC. The solvent was evaporated under reduced pressure and the residue purified by column chromatography.

6,7-Dicarbomethoxy-5-methyl-1-phenyl-8-oxabicyclo[3.2.1]oct-6-en-2-one Diazodione **12** and DMAD. Column chromatography (SiO₂, 10:1 petrol:Et₂O) gave the title compound as a white solid: mp 86–87 °C (petrol:Et₂O); R_f = 0.65 (1:1 petrol:Et₂O); IR (KBr disc) cm⁻¹ 1733, 1718, 1651, 1435, 1323, 1305m cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.49–7.46 (2H, m), 7.39–7.35 (3H, m), 3.84 (3H, s), 3.71 (3H, s), 2.99 (1H, ddd, J = 17.5, 9, 9 Hz), 2.64 (1H, ddd, J = 17.5, 7, 2 Hz), 2.47–2.36 (2H, m), 1.76 (3H, s); ¹³C NMR (100 MHz, CDCl₃) δ 197.6, 163.5, 162.4, 145.4, 139.9, 132.2, 128.5, 127.9, 126.8, 92.2, 86.9, 52.6, 35.3, 34.1, 22.8; MS (APCI) m/z 353 (M + Na⁺, 100); HRMS (ES) calcd for C₁₈H₁₉O₆ 331.1181, found 331.1177 (M + H⁺). Anal. Calcd for C₁₈H₁₈O₆: C, 65.45; H, 5.5. Found: C, 65.5; H, 5.5.

6,7-Dicarbomethoxy-5-methyl-1-(4-nitrophenyl)-8-oxabicyclo[3.2.1]oct-6-en-2-one

Diazodione **13** and DMAD. Column chromatography (SiO₂, 3:1 petrol:Et₂O) gave the title compound as a yellow solid: mp 120–121 °C (petrol:Et₂O); R_f = 0.75 (Et₂O); IR (KBr disc) 2955, 1745, 1719, 1527, 1347, 1264 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.21 (2H, d, J = 9 Hz), 7.70 (2H, d, J = 9 Hz), 3.85 (3H, s), 3.72 (3H, s), 3.00 (1H, ddd, J = 17.5, 9, 9 Hz), 2.65 (1H, ddd, J =

17.5, 7, 2 Hz), 2.49–2.37 (2H, m), 1.77 (3H, s); ^{13}C NMR (100 MHz, CDCl_3) δ 196.5, 162.9, 162.1, 147.8, 143.6, 141.1, 139.1, 128.1, 122.8, 91.4, 87.5, 52.8, 35.2, 33.8, 22.7; MS (CI, NH_3) m/z 393 ($\text{M} + \text{NH}_4^+$, 100), 363 (68), 268 (26); HRMS (ES) calcd for $\text{C}_{18}\text{H}_{21}\text{N}_2\text{O}_8$ 393.1298, found 393.1296 ($\text{M} + \text{NH}_4^+$). Anal. Calcd for $\text{C}_{18}\text{H}_{17}\text{NO}_8$: C, 57.6; H, 4.6; N, 3.7. Found: C, 57.7; H, 4.7; N, 3.6.

7-(4-Methoxyphenyl)-5-methyl-1-phenyl-8-oxabicyclo[3.2.1]oct-6-en-2-one (19)

Diazodione **12** and 4-methoxyphenylacetylene (**16**). Column chromatography (SiO_2 , 10:1 petrol: Et_2O) gave **19** as a pale yellow solid: mp 139–140 °C (petrol: EtOAc); R_f = 0.55 (1:1 petrol: Et_2O); IR (KBr disc) 2927, 1715, 1606, 1514, 1248, 1180s cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.44–7.41 (2H, m), 7.31–7.27 (3H, m), 7.18 (2H, d, J = 9 Hz), 6.74 (2H, d, J = 9 Hz), 6.42 (1H, s), 3.75 (3H, s), 2.88–2.74 (2H, m), 2.41 (1H, dd, J = 13.5, 8.5, 8.5), 2.05 (1H, ddd, J = 13.5, 8.5, 2 Hz), 1.61 (3H, s); ^{13}C NMR (100 MHz, CDCl_3) δ 203.7, 159.3, 143.3, 135.2, 133.3, 129.2, 128.4, 128.1, 124.4, 113.7, 95.0, 84.4, 55.2, 35.0, 34.8, 24.5; MS (CI, NH_3) m/z 338 ($\text{M} + \text{NH}_4^+$, 100), 321 ($\text{M} + \text{H}^+$, 28), 176 (31), 160 (34); HRMS (ES) calcd for $\text{C}_{21}\text{H}_{21}\text{O}_3$ 321.1490, found 321.1491 ($\text{M} + \text{H}^+$). Anal. Calcd for $\text{C}_{21}\text{H}_{20}\text{O}_3$: C, 78.7; H, 6.3. Found: C, 78.85; H, 6.4.

5-Methyl-1,7-diphenyl-8-oxabicyclo[3.2.1]oct-6-en-2-one (20) Diazodione **12** and phenylacetylene (**17**). Column chromatography (SiO_2 , 20:1 petrol: Et_2O) gave **20** as a white solid: mp 122–123 °C (petrol: EtOAc); R_f = 0.65 (1:1 petrol: Et_2O); IR (KBr disc) 2921, 2854, 1716, 1448, 1373, 1187 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.42–7.40 (2H, m), 7.31–7.20 (8H, m), 6.54 (1H, s), 2.92–2.74 (2H, m), 2.43 (1H, ddd, J = 13.5, 8.5, 8.5 Hz), 2.07 (1H, ddd, J = 13.5, 8.5), 1.63 (3H, s); ^{13}C NMR (100 MHz, CDCl_3) δ 203.5, 144.0, 135.4, 135.0, 132.1, 129.2, 128.5, 128.3, 128.1, 128.0, 126.7, 95.1, 84.5, 35.0, 34.7, 24.4; MS (CI, NH_3) m/z 308 ($\text{M} + \text{NH}_4^+$, 100),

291 ($M + H^+$, 35); HRMS (ES) calcd for $C_{20}H_{22}NO_2$ 308.1651, found 308.1649 ($M + NH_4^+$).

Anal. Calcd for $C_{20}H_{18}O_2$: C, 82.7; H, 6.25. Found: C, 82.6; H, 6.25.

5-Methyl-7-(4-nitrophenyl)-1-phenyl-8-oxabicyclo[3.2.1]oct-6-en-2-one (21) Diazodione **12** and 4-nitrophenylacetylene (**18**). Column chromatography (SiO_2 , 10:1 $\rightarrow$ 5:1 petrol:Et₂O) gave **21** as a yellow solid: mp 108–109 °C (petrol:Et₂O); R_f = 0.35 (1:1 petrol:Et₂O); IR (KBr disc) 2931, 1716, 1593, 1512, 1448, 1340 cm^{-1} ; 1H NMR (400 MHz, $CDCl_3$) δ 8.06 (2H, d, J = 9 Hz), 7.41 (2H, d, J = 9 Hz), 7.38–7.35 (2H, m), 7.32–7.28 (3H, m), 6.76 (1H, s), 2.93–2.80 (2H, m), 2.49–2.42 (1H, m), 2.11 (1H, ddd, J = 13.5, 7.5, 4.5 Hz), 1.65 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.3, 147.0, 142.5, 139.6, 138.4, 134.2, 129.0, 128.9, 128.4, 127.4, 123.6, 95.1, 84.7, 35.2, 34.2, 24.3; MS (CI, NH_3) m/z 353 ($M + NH_4^+$, 82), 323 (97), 306 (79), 209 (100); HRMS (ES) calcd for $C_{20}H_{21}N_2O_4$ 353.1501, found 353.1497 ($M + NH_4^+$). Anal. Calcd for $C_{20}H_{17}NO_4$: C, 71.6; H, 5.1; N, 4.2. Found: C, 71.7; H, 5.1; N, 4.2.

7-(4-Methoxyphenyl)-5-methyl-1-(4-nitrophenyl)-8-oxabicyclo[3.2.1]oct-6-en-2-one (22) Diazodione **13** and 4-methoxyphenylacetylene (**16**). Column chromatography (SiO_2 , 3:1 petrol:Et₂O) gave **22** as a pale yellow oil: R_f = 0.40 (1:1 petrol:Et₂O); IR (neat) 2928, 1717, 1605, 1513, 1346, 1249, 1181 cm^{-1} ; 1H NMR (400 MHz, $CDCl_3$) δ 8.13 (2H, d, J = 9 Hz), 7.67 (2H, d, J = 9 Hz), 7.07 (2H, d, J = 9 Hz), 6.75 (2H, d, J = 9 Hz), 6.41 (1H, s), 3.75 (3H, s), 2.91 (1H, ddd, J = 18.5, 8.5, 8.5 Hz), 2.75 (1H, ddd, J = 18.5, 8.5, 2 Hz), 2.43 (1H, ddd, J = 13.5, 8.5, 8.5 Hz), 2.10 (1H, ddd, J = 13.5, 8.5, 2 Hz), 1.64 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.5, 159.6, 147.5, 143.5, 142.3, 133.6, 130.1, 128.1, 123.8, 123.0, 113.9, 93.5, 85.4, 55.2, 34.7, 34.6, 24.3; MS (CI, NH_3) m/z 383 ($M + NH_4^+$, 100), 336 (24), 90 (63), 60 (57); HRMS (ES) calcd for $C_{21}H_{23}N_2O_5$ 383.1607, found 383.1614 ($M + NH_4^+$).

5-Methyl-1-(4-nitrophenyl)-7-phenyl-8-oxabicyclo[3.2.1]oct-6-en-2-one (23) Diazodione **13** and phenylacetylene (**17**). Column chromatography (SiO_2 , 10:1 petrol:Et₂O) gave **23** as a yellow

solid: mp 86–87 °C (petrol:Et₂O); *R*_f = 0.50 (1:1 petrol:Et₂O); IR (KBr disc) 2931, 1716, 1521, 1351 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.12 (2H, d, *J* = 9 Hz), 7.68 (2H, d, *J* = 9 Hz), 7.25–7.20 (3H, m), 7.16–7.13 (2H, m), 6.52 (1H, s), 2.94 (1H, ddd, *J* = 18.5, 8.5, 8.5 Hz), 2.76 (1H, ddd, *J* = 18.5, 8.5, 2 Hz), 2.46 (1H, ddd, *J* = 13.5, 8.5, 8.5 Hz), 2.07 (1H, ddd, *J* = 13.5, 8.5, 2 Hz), 1.63 (3H, s); ¹³C NMR (100 MHz, CDCl₃) δ 202.3, 147.5, 144.2, 142.0, 135.6, 131.6, 130.0, 128.5, 126.7, 123.0, 93.5, 85.5, 34.6, 24.2; MS (CI, NH₃) *m/z* 353 (*M* + NH₄⁺, 98), 306 (85), 192 (100); HRMS (ES) calcd for C₂₀H₂₁N₂O₄ 353.1501, found 353.1490 (*M* + NH₄⁺). Anal. Calcd for C₂₀H₁₇NO₄: C, 71.6; H, 5.1; N, 4.2. Found: C, 71.1; H, 5.1; N, 4.7.

5-Methyl-1,7-bis(4-nitrophenyl)-8-oxabicyclo[3.2.1]oct-6-en-2-one (24) Diazodione **13** and 4-nitrophenylacetylene (**18**). Column chromatography (SiO₂, 5:1 petrol:Et₂O) gave **24** as a yellow oil: *R*_f = 0.15 (1:1 petrol:Et₂O); IR (neat) 2931, 1719, 1599, 1519, 1349, 1110 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.13 (2H, d, *J* = 9 Hz), 8.07 (2H, d, *J* = 9 Hz), 7.64 (2H, d, *J* = 9 Hz), 7.34 (2H, d, *J* = 9 Hz), 6.76 (1H, s), 2.95–2.81 (2H, m), 2.48 (1H, ddd, *J* = 14, 8, 8 Hz), 2.15 (1H, ddd, *J* = 14, 7, 3.5 Hz), 1.68 (3H, s); ¹³C NMR (100 MHz, CDCl₃) δ 202.1, 147.8, 147.3, 142.5, 141.3, 139.6, 137.9, 130.0, 127.4, 123.8, 123.3, 93.4, 85.7, 34.8, 34.1, 24.1; MS (CI, NH₃) *m/z* 398 (*M* + NH₄⁺, 30), 272 (33), 114 (72), 94 (100); HRMS (ES) calcd for C₂₀H₂₀N₃O₆ 398.1352, found 398.1360 (*M* + NH₄⁺).

Chiral HPLC Conditions

Conditions using Whelk-O chiral column were developed by Eric Hortense, GlaxoSmithKline, Stevenage.

Cycloadduct	Column	Eluant	Flow (cm ³ min ⁻¹)	Wavelength (nm)	Retention Times (min)
10	OJ	90:10 hexane:EtOH	0.5	254	18.7 20.4
11	OD	80:20 hexane:EtOH	1	215	12.7 15.1
AD	80:20 heptane:EtOH	0.5	254	9.1 10.3
Whelk-O 1	90:10 heptane:EtOH	1	215	18.3 21.1
19	AD	95:5 heptane:EtOH	0.7	254	9.8 11.6
20	AD	95:5 heptane:EtOH	1	215	5.1 6.4

<p>21</p>	OD	90:10 heptane: <i>i</i> PrOH	1	254	10.9 12.4
<p>22</p>	AD	95:5 hexane: <i>i</i> PrOH	1	215	13.8 16.8
<p>23</p>	AD	90:10 heptane:EtOH	1	254	8.5 10.9
<p>24</p>	AD	90:10 heptane:EtOH	1	254	27.4 32.5

Cycloaddition reactions with DMAD

Scheme S3

Entry	Diazodione	Catalyst	Temp.	Solvent	Yield (%)	<i>ee</i> ^a (%)	$[\alpha]_D^{T\ b}$
1	12	Rh ₂ (OAc) ₄	rt	CH ₂ Cl ₂	77	-	-
2	12	Rh ₂ (<i>S</i> -DOSP) ₄	rt	hexane	73	6	+27.6
3	12	Rh ₂ (<i>R</i> -BNP) ₄	rt	hexane	48	1	-
4	12	Rh ₂ (<i>R</i> -DDBNP) ₄	rt	hexane	56	2	-
5	12	Rh ₂ (<i>S</i> -BPTV) ₄	rt	CH ₂ Cl ₂	57	6	-31.0
6	12	Rh ₂ (<i>S</i> -BPTV) ₄	rt	PhCF ₃	73	36	+103.6
7	12	Rh ₂ (<i>S</i> -BPTV) ₄	32 °C	PhCF ₃	70	31	+154.9
8	13	Rh ₂ (OAc) ₄	rt	CH ₂ Cl ₂	80	-	-
9	13	Rh ₂ (<i>R</i> -BNP) ₄	rt	hexane	25	1	-
10	13	Rh ₂ (<i>S</i> -BPTV) ₄	rt	CH ₂ Cl ₂	33	1	-
11	13	Rh ₂ (<i>S</i> -BPTV) ₄	rt	PhCF ₃	47	3	-
12	13	Rh ₂ (<i>S</i> -BPTV) ₄	32 °C	PhCF ₃	33	1	-

^a Determined by chiral HPLC. ^b c = 1.0-1.13 in CHCl₃, T = 22-25 °C

Table S1. Effect of experimental conditions on the cycloadditions of diazodiones **12** and **13** with DMAD.

10

10

12

12

13

Density Functional Theory Calculations

π -HOMO and LUMO energies and orbital coefficients (obtained from density functional theory (DFT) calculations with geometries optimised at the B3LYP/6-31G(d) level²⁴), in the absence of a catalyst, are presented in Table S2. The energy gaps for both interactions are also included.

	Coefficients ^a				Energies (Hartrees)		Energy Gaps (Hartrees)			
	HOMO		LUMO		HOMO	LUMO	14		15	
	C-1	C-2	C-1	C-2			LU _a -HO _d	LU _d -HO _a	LU _a -HO _d	LU _d -HO _a
14	-0.29	0.34	0.44	0.16	-0.18	-0.09	-	-	-	-
15	-0.28	0.35	0.45	0.13	-0.21	-0.11	-	-	-	-
a16	-0.15	-0.27	0.17	-0.24	-0.22	-0.03	0.15	0.13	0.18	0.11
a17	0.21	0.32	0.15	-0.24	-0.24	-0.04	0.14	0.15	0.16	0.13
a18	0.24	0.33	0.04	-0.15	-0.27	-0.12	0.07	0.18	0.09	0.16

^a All for 2p_z AO. **d** = dipole, **a** = acetylene. For **d** C-1 represents original carbonyl C and C-2 original diazo C; for **a** C-1 represents substituted C and C-2 unsubstituted C.

Table S2. DFT calculations: frontier orbital coefficients and energies.

Compound 14: optimisation archive

```
I\1\GINC-CLUSTER13\FOpt\RB3LYP\6-31+G(d)\C12H12O2\GUY\10-Jul-2001\0\#
B3LYP/6-31+G* OPT=(CALCFC)\dipole_gh #B3LYP/6-31+g* optimization\0,1
\C,1.0913131175,-0.0330958578,-1.7958156524\C,1.0725938177,0.009153398
9,-0.3818736392\C,2.3150548531,0.0555277415,0.2925482491\C,3.511423888
2,0.0662141459,-0.4246714582\C,3.5156029392,0.0315392334,-1.8218781061
\C,2.2933978347,-0.0182093833,-2.5000115841\C,-0.1850612748,-0.0047986
761,0.3565425828\O,-1.2947830923,0.0755795635,-0.4625367738\C,-2.53503
52375,-0.0929845607,-0.1375586938\C,-2.8219583264,-0.4874943738,1.2652
949867\C,-1.864457055,0.236101063,2.2174713151\C,-0.4043384271,0.06858
278,1.7730496865\C,-3.5378463478,0.0425105835,-1.2273291512\O,0.497985
6785,0.0720086062,2.6246314533\H,-2.636757544,-1.5788389367,1.33964021
28\H,-3.8763295413,-0.3256120579,1.5120375905\H,-1.9543072362,-0.14787
89154,3.2365976657\H,-2.0916171625,1.3127797412,2.2535574351\H,-3.0454
10069,0.2130343688,-2.1881449736\H,-4.1570407051,-0.8641973354,-1.2984
251071\H,-4.2276731835,0.8773146571,-1.0347814355\H,2.323997629,0.0818
```

798043,1.3747739671\H,4.4517473792,0.1029486142,0.1205974002\H,4.45243
34986,0.0392414834,-2.3729866\H,2.2735548659,-0.0502626439,-3.58708966
6\H,0.1576426885,-0.079390704,-2.3471451374\\Version=x86-Linux-G98RevA
.7\HF=-614.9115795\RMSD=5.677e-09\RMSF=2.639e-06\Dipole=-2.5308233,-0.
1176325,-0.9725641\PG=C01 [X(C12H12O2)]\@

Compound 14: frequency calculation archive

1\1\GINC-CLUSTER16\Freq\RB3LYP\6-31+G(d)\C12H12O2\GUY\11-Jul-2002\1\#\n
B3LYP/6-31+G* FREQ=NORAMAN GEOM=CHECKPOINT\dipole_gh\0,1\C\C,1,cc2\O
,2,oc3,1,occ3\C,3,co4,2,coc4,1,dih4,0\C,4,cc5,3,cco5,2,dih5,0\C,5,cc6,
4,ccc6,3,dih6,0\C,2,cc7,3,cco7,4,dih7,0\C,7,cc8,2,ccc8,3,dih8,0\C,8,cc
9,7,ccc9,2,dih9,0\C,9,cc10,8,ccc10,7,dih10,0\C,10,cc11,9,ccc11,8,dih11
,0\C,11,cc12,10,ccc12,9,dih12,0\C,4,cc13,3,cco13,2,dih13,0\O,1,oc14,2,
occ14,7,dih14,0\H,5,hc15,4,hcc15,3,dih15,0\H,5,hc16,4,hcc16,3,dih16,0\
H,6,hc17,5,hcc17,4,dih17,0\H,6,hc18,5,hcc18,4,dih18,0\H,13,hc19,4,hcc1
9,3,dih19,0\H,13,hc20,4,hcc20,3,dih20,0\H,13,hc21,4,hcc21,3,dih21,0\H,
12,hc22,7,hcc22,8,dih22,0\H,11,hc23,12,hcc23,7,dih23,0\H,10,hc24,11,hc
c24,12,dih24,0\H,9,hc25,8,hcc25,7,dih25,0\H,8,hc26,7,hcc26,12,dih26,0\
\cc2=1.435256\oc3=1.381606\occ3=117.349\co4=1.293155\coc4=127.863\dih4
=-17.2\cc5=1.485247\cco5=117.211\dih5=-3.343\cc6=1.532005\ccc6=109.929
\dih6=37.796\cc7=1.458475\cco7=113.073\dih7=169.856\cc8=1.414697\ccc8=
121.141\dih8=-6.191\cc9=1.393241\ccc9=121.082\dih9=179.928\cc10=1.3986
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3,-0.00029917,0.00007217,-0.00038767,-0.00028892,-0.00000469,-0.000893
02,-0.00037629,0.00008757,0.00030337,-0.00013042,-0.00009164,-0.000050
29,0.00001327,-0.00000860,-0.00001656,-0.00001631,0.00003267,0.0000229
9,-0.00139918,0.00114442,0.00394127,0.00039786,-0.00009049,0.00072772,
0.00178365,0.00059722,-0.00091716,-0.00084364,0.00050769,0.00034111,-0
.29631772,0.02851766,-0.09375925,-0.01880441,0.00238060,-0.01044937,-0
.00003361,0.00002692,0.00005922,0.00026542,-0.00003249,0.00028466,0.00
002426,0.00002905,0.00002770,-0.00000679,-0.00000197,0.00001646,-0.000
01222,0.00000004,0.00001963,-0.00002053,-0.00002503,0.00000131,0.00001
087,0.00000140,-0.00000321,-0.00003193,0.00001228,-0.00002829,-0.00003
447,-0.00001060,-0.00002278,0.00098672,-0.00062864,0.00015555,0.314610
88,0.00004219,0.00001135,0.00005108,0.00010265,0.00040060,0.00012936,0
.00007454,-0.00019671,-0.00001046,0.00003597,-0.00003446,-0.00000133,0
.00000112,0.00000886,0.00000354,0.00000753,-0.00001401,-0.00000212,0.0
0116076,0.00719502,-0.00073100,-0.00010568,-0.00052673,-0.00016149,0.0
0067429,0.00672877,-0.00026496,-0.00049406,0.00321445,-0.00041620,0.02
851743,-0.04005599,0.00948425,0.00318893,0.00281476,0.00152938,0.00000
398,0.00000942,-0.00001229,-0.00003403,0.00003231,-0.00003136,-0.00000

311,-0.00001055,-0.00000420,-0.00000008,0.00000039,-0.00000258,0.00000
214,0.00000188,-0.00000494,-0.00000531,-0.00000047,0.00000296,-0.00000
046,0.00000080,0.00000025,0.000000672,-0.00000542,0.00000298,0.00000364
,-0.00000034,0.00000650,-0.00065497,-0.00432172,0.00016207,-0.03186304
,-0.02932510,0.00008893,0.00000343,0.00014525,0.00016222,0.00004702,0.0
0070792,0.00069088,-0.00011155,-0.00014911,-0.00005920,0.00001918,0.00
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001699,0.00354494,-0.00071405,-0.00232785,0.00066157,-0.00009439,-0.00
092913,0.00027009,-0.00041693,-0.00599681,-0.03082820,0.00342722,-0.00
612435,-0.09385488,0.00946922,-0.09701357,0.01995877,-0.00223262,0.010
98051,0.00002376,-0.00000772,-0.00001108,-0.00015494,0.00001116,-0.000
05409,0.00000671,0.00000822,0.00000944,-0.00000112,-0.00000089,-0.0000
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798,-0.00000944,-0.00014690,0.00000573,-0.00002681,0.00000264,0.000203
60,0.00010457,-0.00004739,-0.00002528,-0.00001272,-0.00000463,0.000012
54,-0.00001320,0.00003924,0.00002176,-0.00006037,-0.00006063,-0.000909
03,-0.00375717,0.00113860,-0.00386430,-0.01754150,0.00297136,0.0212518
1,-0.22349861,0.02674274,0.13465811,0.00770350,-0.00077708,-0.00489207
,0.00109493,0.00061374,-0.00150671,-0.00000663,0.00001004,-0.00000312,
0.00006918,-0.00002741,0.00010136,0.00001081,0.00000521,0.00001042,-0.
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0,-0.00000488,-0.00010033,0.00007016,-0.00003820,0.00013305,-0.0000164
7,0.00001165,-0.00058331,-0.00002262,0.00121374,0.00646004,0.00026549,
0.00217195,0.00191471,-0.00227653,0.02670122,-0.03755274,-0.02009167,0.
.00017048,0.00247289,-0.00010906,0.00043255,0.00666604,-0.00007967,0.0
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353,-0.00374424,0.00009189,-0.02960310,0.02836571,-0.00024666,-0.00000
087,-0.00022452,-0.00003674,0.00005417,0.00032946,-0.00015175,-0.00000
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.01103263,0.13472432,-0.02019453,-0.17099375,0.02645463,-0.00365533,-0.
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0.00003722,0.00039121,-0.00004306,-0.00013941,-0.00001538,-0.00001583,
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0.00003009,0.00000109,0.00011785,-0.00357849,0.00151576,0.00290118,0.0
0774399,-0.00003469,0.02536964,-0.06793562,0.00278547,-0.04716995,0.00
032092,-0.00049656,-0.03070163,-0.00550927,0.00147741,-0.00106954,-0.0
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7514,-0.00000281,-0.00006655,0.00000102,0.00000687,0.00000463,-0.00000
157,0.00000087,0.00000433,-0.00003279,-0.00000240,0.00002221,-0.000009
17,-0.00000465,0.00000447,-0.00000914,-0.00000340,-0.00000269,-0.00000
971,-0.00000059,-0.00001029,-0.00000753,-0.00000025,-0.00001255,0.0001
2458,-0.00015039,0.00000550,-0.00015229,-0.00000589,-0.00162967,0.0009
7089,-0.00056423,0.00056932,0.06756400,0.00001520,-0.00019967,-0.00003
109,-0.00004397,0.00036337,-0.00010162,-0.00006609,0.00011930,0.000041
28,0.00003361,-0.00000891,-0.00001257,-0.00000980,-0.00000432,0.000013
25,0.00000837,0.00000029,-0.00001032,0.00144414,0.00720400,-0.00063507
,-0.00091481,0.00263195,-0.00358498,0.00297783,-0.03617266,-0.00196928
,-0.00022265,0.00304701,0.00343949,0.00142320,0.00665970,0.00002922,0.0
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0413,-0.00000613,0.00000178,0.00000258,0.00001477,-0.00000101,0.000007
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138401,0.00035577,-0.00000393,0.00061029,0.00002791,-0.00002671,-0.000
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004353,0.00001167,-0.00000073,-0.00001721,0.00002532,0.00000495,-0.000
02751,0.00001995,0.00002298,-0.00000191,-0.00000194,0.00000261,0.00001
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,-0.00003136,0.00003165,-0.00002133,0.00009482,-0.00003694,-0.00049429
,-0.00034112,0.00015869,0.00087018,0.05071707,0.00238772,0.34824689,0.
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6,0.00000932,-0.00001995,0.00001913,0.00001649,0.00000118,-0.00012134,
0.00000185,-0.00001418,0.00005710,-0.00002303,0.00000452,0.00004790,-0
.00000744,-0.00000123,-0.00021731,-0.00001453,0.00017455,-0.00007581,-
0.00012580,-0.00005179,-0.00098699,0.00019662,-0.00057745,0.00099955,-
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147030,-0.03853107,0.01057365,0.00322847,0.00251311,0.00183080,0.00131
116,0.00713418,-0.00073717,-0.00005601,-0.00059349,-0.00026611,0.00027
327,0.00577827,-0.00025544,-0.00000360,0.00017380,-0.00001084,0.000089
06,-0.00000334,0.00007142,0.00000142,-0.00006585,-0.00006992,0.0000004
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, -0.00000087,0.00000620,-0.00002813,0.00015507,-0.00000923,0.00001415,
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.00035664,0.00008931,-0.00067906,-0.00427781,0.00009758,-0.03512808,0.
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003799,-0.02976472,0.00359738,-0.00571862,-0.09666953,0.01062017,-0.09
873080,0.02020273,-0.00231226,0.01099453,0.00306911,-0.00061706,-0.002
12952,0.00054050,-0.00008344,-0.00090231,0.00081140,-0.00040032,-0.006
24740,-0.00008448,-0.00005122,-0.00017342,0.00063599,-0.00008094,0.000
36927,-0.00003914,-0.00006726,-0.00003152,-0.00001301,0.00000915,0.000
06329,-0.00000033,0.00000849,0.00001299,0.00000484,0.00000218,-0.00001
638,0.00013838,0.00001446,0.00012535,0.00002691,0.00000208,0.00006313,
0.00002515,0.00002222,0.00006831,-0.00177543,0.00022324,-0.00016144,-0.
.00007325,0.00004016,0.00013105,0.00101025,-0.00011639,0.00035263,-0.0
0031138,0.00016064,0.00105467,0.10236598,-0.01106906,0.10176793\0.000
01331,0.00001569,0.00000248,-0.00000504,-0.00000708,-0.00000976,0.0000
1097,0.00001166,0.00000514,-0.00000431,-0.00000507,0.00000369,0.000006
15,0.00000332,0.00000842,-0.00000229,-0.00000487,-0.00000216,-0.000003
42,-0.00002691,-0.00000924,-0.00000085,0.00001962,0.00001455,-0.000001
90,-0.00000857,-0.00003689,0.00000689,0.00000550,-0.00000096,0.0000232
4,-0.00000280,0.00000034,-0.00003020,-0.00000088,0.00004568,-0.0000004
5,-0.00000216,-0.00000278,0.00000153,0.00000102,-0.00000256,0.00000064
,0.00000118,0.00000360,0.00000371,0.00000185,0.00000333,0.00000198,-0.
00000079,-0.00000393,0.00000434,-0.00000022,0.00000209,-0.00000218,-0.
00000086,0.00000668,0.00000253,-0.00000034,0.00000772,-0.00000288,-0.0
0000095,0.00000362,0.00001091,0.00000046,-0.00001280,-0.00000207,0.000
00331,-0.00001680,-0.00001644,0.00000089,-0.00001184,-0.00001764,0.000
00278,0.00000364,0.00000349,-0.00000576,-0.00000126\\\@

Compound 15: optimisation archive

1\1\GINC-CLUSTER2\FOpt\RB3LYP\6-31+G(d)\C12H11N1O4\GUY\17-Dec-2001\0\ \#B3LYP/6-31+G* OPT\dipole_no2 #B3LYP/6-31+g* optimization\0,1\C,1.01 2284777,-0.1007857579,-2.425725762\C,0.9771077792,-0.116076263,-0.987 4898226\O,2.1933914375,-0.1015069512,-0.3184001366\C,3.3573207327,-0.3 776302262,-0.7991773629\C,3.4300057685,-0.822131445,-2.2147189281\C,2. 4075785824,-0.0557283426,-3.0609491686\C,-0.1586993134,0.0114352845,-0 .0991872545\C,0.009964606,0.0463036378,1.3099721077\C,-1.074840333,0.1 678691396,2.1641314727\C,-2.36362125,0.2520265897,1.627713994\C,-2.567 5209424,0.2150459464,0.2453000279\C,-1.4799942007,0.0957771726,-0.6095 099393\N,-3.5060253605,0.3762147006,2.524642494\O,-4.6342605724,0.4455 805757,2.0243578105\C,4.5086466666,-0.2810996842,0.135658999\O,0.00715 53172,-0.0598417773,-3.1467937931\O,-3.2886707538,0.4066268054,3.74240 06648\H,3.1678943427,-1.8990435786,-2.2253849152\H,4.4520356929,-0.740 8464187,-2.5980615201\H,2.3355630473,-0.4741424989,-4.0676776168\H,2.7 030115555,0.9989466075,-3.1668735052\H,4.170117119,-0.0715492755,1.153 2265208\H,5.084709933,-1.2174142446,0.1307159628\H,5.2020142891,0.5139 590719,-0.1753492942\H,-1.6331087657,0.0668493494,-1.6803076778\H,-3.5 750249208,0.2809568954,-0.1485222896\H,-0.9389515297,0.1953619459,3.23 89103846\H,1.0035960957,-0.023486289,1.7381999527\Version=x86-Linux-G 98RevA.7\HF=-819.4281066\RMSD=5.853e-09\RMSF=5.607e-06\Dipole=4.949617 3,-0.5365661,-1.0653808\PG=C01 [X(C12H11N1O4)]\@

Compound 15: frequency calculation archive

1\1\GINC-CLUSTER17\Freq\RB3LYP\6-31+G(d)\C12H11N1O4\GUY\13-Jul-2002\1\ \#B3LYP/6-31+G* FREQ=NORAMAN\dipole_gno2\0,1\C\C,1,cc2\C,2,cc3,1,ccc 3\C,3,cc4,2,ccc4,1,dih4,0\C,4,cc5,3,ccc5,2,dih5,0\C,5,cc6,4,ccc6,3,dih 6,0\C,2,cc7,3,ccc7,4,dih7,0\C,7,cc8,2,ccc8,3,dih8,0\C,8,cc9,7,ccc9,2,d ih9,0\C,9,cc10,8,ccc10,7,dih10,0\C,10,cc11,9,ccc11,8,dih11,0\O,11,oc12 ,10,occ12,9,dih12,0\O,8,oc13,7,occ13,12,dih13,0\C,11,cc14,12,cco14,7,d ih14,0\N,5,nc15,4,ncc15,3,dih15,0\O,15,on16,5,onc16,4,dih16,0\O,15,on1 7,5,onc17,4,dih17,0\H,10,hc18,11,hcc18,12,dih18,0\H,10,hc19,11,hcc19,1 2,dih19,0\H,9,hc20,8,hcc20,7,dih20,0\H,9,hc21,8,hcc21,7,dih21,0\H,14,h c22,11,hcc22,12,dih22,0\H,14,hc23,11,hcc23,12,dih23,0\H,14,hc24,11,hcc 24,12,dih24,0\H,1,hc25,2,hcc25,7,dih25,0\H,6,hc26,5,hcc26,4,dih26,0\H, 4,hc27,3,hcc27,2,dih27,0\H,3,hc28,2,hcc28,7,dih28,0\cc2=1.418931\cc3= 1.419645\ccc3=117.786\cc4=1.386062\ccc4=121.39\dih4=-0.439\cc5=1.39849 3\ccc5=119.351\dih5=0.289\cc6=1.397859\ccc6=120.808\dih6=-0.005\cc7=1. 447549\ccc7=121.203\dih7=-179.98\cc8=1.438747\ccc8=129.175\dih8=-176.4 94\cc9=1.533748\ccc9=115.885\dih9=171.4\cc10=1.532591\ccc10=111.317\di h10=33.404\cc11=1.485471\ccc11=110.114\dih11=-50.587\oc12=1.289233\occ 12=117.621\dih12=37.177\oc13=1.237699\occ13=124.255\dih13=-177.128\cc1 4=1.486199\cco14=116.802\dih14=179.804\nc15=1.457735\ncc15=119.428\dih 15=179.832\on16=1.237377\onc16=118.032\dih16=0.202\on17=1.236127\onc17 =118.102\dih17=-179.833\hc18=1.108402\hcc18=106.758\dih18=-80.811\hc19 =1.094579\hcc19=110.928\dih19=163.153\hc20=1.092592\hcc20=108.084\dih2 0=155.77\hc21=1.100382\hcc21=108.196\dih21=-88.434\hc22=1.092684\hcc22 =110.991\dih22=5.443\hc23=1.099345\hcc23=110.352\dih23=126.719\hc24=1. 099819\hcc24=110.945\dih24=-115.48\hc25=1.082075\hcc25=119.083\dih25=- 0.195\hc26=1.083745\hcc26=119.562\dih26=179.947\hc27=1.083684\hcc27=12 1.015\dih27=-179.907\hc28=1.08423\hcc28=119.956\dih28=-0.02\Version=x 86-Linux-G98RevA.7\HF=-819.428178\RMSD=1.764e-09\RMSF=1.166e-05\Dipole =-2.7884479,0.1192815,4.2573973\DipoleDeriv=-0.3641998,0.0017046,0.328

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3597,-0.00000432,-0.00000068,0.00000034,-0.00000725,0.00000369,-0.0000
0811,0.00000447,0.00000024,-0.00000386,0.00000020,0.00000041,-0.000002
51,-0.00000849,-0.00000255,0.00000213,-0.00001129,-0.00000270,-0.00000
452,-0.00000346,-0.00000431,0.00000158,0.00001640,0.00000568,-0.000009
56,0.00000936,0.00000102,0.00000607,-0.00000344,-0.00000086,0.00000464
,0.00000042,-0.00000293,0.00000199\\\\@

Compound a16: optimisation archive

1\1\GINC-CLUSTER8\SP\RB3LYP\6-31+G(d)\C9H8O1\GUY\22-Aug-2001\0\#B3LYP
/6-31+G* GEOM=CHECKPOINT GUESS=READ POP=FULL\3_meophenyl\0,1\C,-0.24
98987862,0,-2.9543100994\C,-0.1957814878,0,-1.5258017338\C,-0.296667
3327,0,-4.1661950786\H,-0.3391640612,0,-5.2325289138\C,-1.3803151271
0,-0.756664013\C,-1.3289235038,0,0.6294003862\C,-0.0900278718,0,1.
2920733789\C,1.0961187318,0,0.5452703724\C,1.0354126265,0,-0.8498448
888\H,-2.3415348043,0,-1.2621064541\H,-2.237447166,0,1.2242388077\O,
-0.1472900662,0,2.6552271864\H,2.0651376426,0,1.0315984636\H,1.95708
68158,0,-1.4244314981\C,1.0705952458,0,3.3906884542\H,0.7800135204,0
,4.4424092958\H,1.6655768072,-0.8970017041,3.1756510695\H,1.665576807
2,0.8970017041,3.1756510695\Version=x86-Linux-G98RevA.7\State=1-A\HF
=-422.9350155\RMSD=2.574e-07\Dipole=0.5440885,0,0.6225268\PG=CS [SG(C
9H6O1),X(H2)]\@

Compound a16: frequency calculation archive

1\1\GINC-CLUSTER16\Freq\RB3LYP\6-31+G(d)\C9H8O1\GUY\10-Jul-2002\0\#B3
LYP/6-31+G* FREQ=NORAMAN GEOM=CHECKPOINT\3_meophenyl\0,1\C,-0.249898
7862,0,-2.9543100994\C,-0.1957814878,0,-1.5258017338\C,-0.2966673327
0,-4.1661950786\H,-0.3391640612,0,-5.2325289138\C,-1.3803151271,0,
-0.756664013\C,-1.3289235038,0,0.6294003862\C,-0.0900278718,0,1.2920
733789\C,1.0961187318,0,0.5452703724\C,1.0354126265,0,-0.8498448888\H,
-2.3415348043,0,-1.2621064541\H,-2.237447166,0,1.2242388077\O,-0.1
472900662,0,2.6552271864\H,2.0651376426,0,1.0315984636\H,1.957086815
8,0,-1.4244314981\C,1.0705952458,0,3.3906884542\H,0.7800135204,0,4.
4424092958\H,1.6655768072,-0.8970017041,3.1756510695\H,1.6655768072,0.
8970017041,3.1756510695\Version=x86-Linux-G98RevA.7\State=1-A\HF=-42
2.9350155\RMSD=5.392e-09\RMSF=5.985e-05\Dipole=0.5440884,0,0.6225267\
DipoleDeriv=-0.1136304,-0.0006424,0.0381119,0.0002733,-0.0193245,0.004
2595,0.049841,-0.0009095,0.609564,-0.1198241,0.0003204,-0.0010787,-0.0
000085,-0.01996,0.0007952,-0.0313295,0.0021488,-0.0148094,-0.2660273,0
.0002649,-0.0210999,-0.0004184,-0.3267632,-0.0048308,-0.0428003,-0.000
9702,-0.8396138,0.2337712,-0.0000885,-0.0007019,-0.0001981,0.2592014,0
.000298,0.0022823,0.0002429,0.2363958,0.1335086,0.0000127,-0.0733239,0
.0002687,-0.1020895,-0.0005331,-0.0334128,-0.0002098,0.1945416,-0.0090
907,0.0001886,-0.3697131,-0.0007302,-0.1581447,0.0015888,-0.0701633,0.
000031,-0.379707,0.1063298,0.0000567,-0.0662677,0.0001444,0.1036847,-0
.0005393,0.2388892,-0.0003095,1.8882251,-0.0069066,0.0003039,0.3524139
,0.0001471,-0.1751032,-0.000012,-0.0728817,-0.0000921,-0.4497875,0.142
8827,0.0000915,0.0532639,-0.0003551,-0.0994908,0.0002523,0.0875075,0.0
000807,0.2007611,-0.0400063,0.0001022,-0.0596046,0.0000018,0.1312819,-
0.0000021,-0.0707915,0.0001023,0.0391182,-0.0130525,-0.000244,0.074058
3,0.0003056,0.1469221,-0.0004912,0.0669539,0.0001514,0.0159051,-0.5513
092,-0.0000361,-0.3567373,-0.0002495,-0.2830451,0.0005556,-0.4213766,-
0.0001045,-2.1568438,-0.0394169,-0.0003666,-0.0899227,0.0001351,0.1462
47,-0.000128,-0.0659976,-0.0002285,0.0279066,-0.0311288,-0.0000044,0.0
677646,0.0003778,0.1315875,-0.0006191,0.0670188,-0.0000307,0.0247902,0
.6404549,0.0004058,0.6589758,-0.0001727,0.3579122,-0.0002027,0.2336181
,0.0002616,0.6839318,0.0477089,-0.0000624,0.0496263,-0.0002807,0.09139
19,0.0004839,-0.013386,-0.0002478,-0.151918,-0.0575939,0.0620472,-0.12
72804,0.0967616,-0.0919972,0.0053854,0.03803,-0.0701643,0.035826,-0.05
7574,-0.0623681,-0.1270773,-0.0967363,-0.0923216,-0.005126,0.0380164,0
.0702231,0.0356892\Polar=98.9702344,0.0055575,61.269731,9.6245289,-0.0
102408,181.136209\PG=CS [SG(C9H6O1),X(H2)]\NImag=0\0.10538227,0.00001
891,0.07902988,0.05064830,0.00031238,1.41252223,-0.07741536,0.00007981
, -0.00775594,0.63195671,-0.00000289,-0.05183286,0.00004318,0.00001586,
0.13378690,-0.00843088,-0.00013272,-0.29675879,0.00848812,-0.00000184,
0.68413405,-0.02938129,-0.00004808,-0.03984250,0.00603311,-0.00000540,

-0.00105447,0.04452012,-0.00003358,-0.03173170,-0.00038501,-0.00008788
0.00561478,0.00019452,0.00006089,0.03721359,-0.03969500,-0.00020178,-
1.05389038,-0.00150275,-0.00004217,-0.02421643,0.05667397,0.00022101,1
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397289,-0.00003050,-0.00000331,0.01025786,0.00010295,-0.00000640,0.003
59206,-0.00022112,0.00000109,0.00090736,-0.01588963,0.00001201,-0.4195
5007,0.01598817,0.00000878,0.41498096,0.00690598,-0.00019114,0.0157818
5,-0.25330353,-0.00003100,0.10338561,-0.00169889,0.00022415,-0.0092351
2,-0.00022041,0.00000277,0.00025138,0.70356836,0.00003105,0.00063727,0
.00004398,-0.00001633,-0.06116368,-0.00010480,-0.00001228,0.00183733,0
.00004781,0.00000396,-0.00004394,-0.00001211,0.00000126,0.13237303,0.0
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88887,-0.00023848,0.00528936,-0.00117428,-0.00001016,-0.00013300,0.044
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826,-0.00000622,0.02326059,0.00013576,0.00006416,-0.00085978,0.0002030
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.00000949,-0.05536956,-0.00001796,0.00002226,0.12294183,0.00235367,-0.
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03,-0.07867304,-0.28311474,0.00001371,-0.03214216,0.70192418,0.0000172
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22,-0.00000635,-0.00001023,-0.00296089,0.00001592,-0.00000721,0.007600
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, -0.01982219,0.00000766,0.01880801,-0.00361299,0.00000539,-0.00390819,
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0548,-0.00000332,-0.00068650,-0.00000466,-0.00000595,-0.00456881,-0.00
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2705,0.00000618,-0.00453439,-0.00007668,-0.00003062,-0.00042763,-0.000
07225,0.00000493,0.00001502,0.02774674,-0.00000764,-0.01214300,0.12958
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714,-0.00002823,0.00041823,0.00473597,-0.00000500,-0.00038773,-0.00002
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32,0.00000473,0.00001116,-0.00000415,0.00446857,-0.00000500,0.00000734
,0.00604426,-0.00000642,0.00000526,-0.04198653,-0.00000991,0.00001348,
0.00860430,-0.00000327,0.00000826,0.00668900,0.00000311,0.00000548,0.0
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06,0.00172738,-0.00000258,0.00320049,-0.00022729,-0.00000008,-0.000907
26,0.00105953,0.00000559,0.00132735,0.09740043,-0.00000629,0.51116212,
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276632,-0.00001246,0.00075874,-0.00000849,0.00000024,-0.00005467,-0.00
102166,0.00001909,-0.00078670,0.00133532,-0.00002028,-0.00049572,0.303
66290,0.00001599,0.00068585,0.00003023,-0.00000577,0.00690145,-0.00005
389,-0.00000767,-0.00017538,0.00001613,0.00000268,-0.00003214,-0.00000
570,-0.00000481,-0.00051011,0.00000993,-0.00000575,0.00512970,-0.00000
717,0.00000035,0.00328258,0.00001085,-0.00000760,-0.03155927,0.0000032
0,0.00000122,0.00177320,-0.00000220,-0.00000223,-0.00083610,-0.0000010
4,0.00000558,0.00007178,-0.00000287,0.00000028,-0.00271826,0.00000153,
0.00000576,0.02304492,-0.00144986,-0.00015104,-0.00031230,0.00127543,-
0.00002636,-0.00469363,0.00008780,0.00017283,-0.00067044,0.00006440,-0
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,-0.00408226,0.00028184,-0.00000100,-0.00078670,0.00144311,-0.00000054
,-0.00131852,0.00525513,0.000000146,-0.00294767,-0.26381467,-0.00000236
 ,0.12603684,-0.00104153,0.00000015,0.00088607,0.00000059,0.00000084,0.
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029497,0.27798836,0.00004358,-0.00372577,0.00006916,-0.00002045,0.0039
1271,-0.00014872,-0.00001842,-0.00012600,0.00006093,0.00000610,0.00024
605,-0.00001685,-0.00000326,0.00577570,0.00001740,-0.00001347,-0.00076
901,-0.00000493,-0.00000336,0.00727507,0.00002214,-0.00002115,0.003442
83,0.00000680,-0.00000450,-0.03648840,-0.00000550,-0.00000735,0.000357
08,-0.00000644,0.00001648,-0.00074597,-0.00000984,0.00000230,-0.000153
79,0.00000682,0.00002364,-0.00414988,0.00001329,0.00000123,0.02509700,
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0.00291293,0.00000138,-0.00123446,-0.00057574,-0.00000487,-0.00050841,
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0.12764405,0.00000149,-0.13796724,-0.00074496,-0.00000006,0.00062004,0.
.00007191,0.00000091,0.00006395,0.00150927,-0.00000188,-0.00134988,-0.
00018350,-0.00000032,0.00106494,-0.13538400,0.00000102,0.14408485,-0.0
0019027,0.00000800,-0.00150837,0.00055759,0.00000595,0.00187399,0.0000
4814,-0.00000305,0.00156916,0.00001080,0.00001389,-0.00016657,-0.00014
893,-0.00001964,-0.00050646,0.00225838,0.00005441,0.00503680,0.0012354
9,-0.00001220,-0.01626753,0.00274942,-0.00000909,0.00950205,-0.0017639
6,0.00002340,-0.00124660,0.00013493,-0.00000016,0.00031701,0.00003898,
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530,-0.00004493,0.,0.00009325,-0.00003243,0.,-0.00019652,0.00007860,0.
,0.00016866,-0.00001934,0.,-0.00004601,-0.00007296,0.,-0.00007793,-0.0
0000796,0.,-0.00001243,-0.00001097,0.,0.00002838,-0.00008713,0.,0.0000
0548,0.00000518,0.,-0.00000976,0.00001978,0.,0.00000665,0.00014700,0.,
0.00007195,-0.00000918,0.,-0.00004458,-0.00003265,0.00003668,-0.000005
65,-0.00003265,-0.00003668,-0.00000565\\@

Compound a17: optimisation archive

1\1\GINC-CLUSTER4\SP\RB3LYP\6-31+G(d)\C8H6\GUY\21-Aug-2001\0\#B3LYP/6-31+G* GEOM=CHECKPOINT GUESS=READ POP=FULL\2_phenyl\0,1\C,0.0033582725,0.,-2.0259719492\C,0.0005566922,0.,-0.5949975944\C,0.0073576733,0.,-3.2381456011\H,0.0096794971,0.,-4.3055614823\C,-1.2147197571,0.,0.1178813093\C,-1.2126536267,0.,1.5122561399\C,-0.0039771796,0.,2.2159516936\C,1.2070072611,0.,1.5161720986\C,1.2135596822,0.,0.1218621577\H,-2.1516709714,0.,-0.4314647659\H,-2.1568162173,0.,2.0508624773\H,-0.0057546604,0.,3.3028250685\H,2.1494123116,0.,2.0578509183\H,2.1522159329,0.,-0.4245617415\Version=x86-Linux-G98RevA.7\State=1-A\HF=-308.4077293\RMSD=2.049e-08\Dipole=-0.0020396,0.,0.2785982\PG=CS [SG(C8H6)]\@

Compound a17: frequency calculation archive

1\1\GINC-CLUSTER20\Freq\RB3LYP\6-31+G(d)\C8H6\GUY\10-Jul-2002\0\#B3LYP/6-31+G* FREQ=NORAMAN GEOM=CHECKPOINT\2_phenyl\0,1\C,0.0033582725,0.,-2.0259719492\C,0.0005566922,0.,-0.5949975944\C,0.0073576733,0.,-3.2381456011\H,0.0096794971,0.,-4.3055614823\C,-1.2147197571,0.,0.1178813093\C,-1.2126536267,0.,1.5122561399\C,-0.0039771796,0.,2.2159516936\C,1.2070072611,0.,1.5161720986\C,1.2135596822,0.,0.1218621577\H,-2.1516709714,0.,-0.4314647659\H,-2.1568162173,0.,2.0508624773\H,-0.0057546604,0.,3.3028250685\H,2.1494123116,0.,2.0578509183\H,2.1522159329,0.,-0.4245617415\Version=x86-Linux-G98RevA.7\State=1-A\HF=-308.4077293\RMSD=8.428e-09\RMSF=8.518e-05\Dipole=-0.0020397,0.,0.2785986\DipoleDeriv=-0.1060489,0.0005572,0.0000259,0.0018975,-0.0155428,-0.0014177,0.0009611,-0.0003614,0.3392473,0.0470522,0.0004238,0.0013901,-0.0051934,-0.0121687,0.0043332,0.0047174,-0.0071027,0.2839566,-0.2585051,-0.0006132,-0.0022502,0.0017411,-0.3113054,-0.00194,-0.0086858,0.0085104,-0.6755557,0.2361424,0.0002018,-0.0000925,0.0004155,0.2539258,-0.0003355,0.0049305,-0.0046902,0.2325453,0.0465821,-0.0028062,0.027116,-0.0002814,-0.0997238,0.0001146,0.0854494,0.0023599,-0.072601,0.0701418,-0.0008002,-0.1016894,0.0000294,-0.1333138,-0.0001752,-0.106464,0.0006619,-0.0152989,-0.0043066,-0.0010645,-0.0006014,0.0004508,-0.1333831,-0.0004515,0.0017257,-0.0002888,0.0281161,0.0687817,-0.000902,0.1050588,-0.0003035,-0.1306705,0.0000987,0.1076206,0.0007643,-0.0152172,0.041119,0.0003065,-0.024426,0.0007259,-0.1042951,-0.0006304,-0.0874097,0.0010499,-0.0715902,-0.0369124,-0.0000492,-0.0596056,0.0008232,0.1334279,-0.0003039,-0.0735921,-0.0000533,0.0326117,-0.0678126,0.0013892,0.0846458,-0.0001668,0.1389659,0.0002419,0.073777,-0.0009872,0.0096366,0.0671315,0.0001633,-0.0000371,-0.0001846,0.1407562,0.0001292,-0.0017186,0.0005595,-0.1169547,-0.0674701,0.0015678,-0.0874847,-0.0002951,0.1392315,0.0003569,-0.0739728,0.0007616,0.0075139,-0.035893,0.0016265,0.0579458,0.0003401,0.1340997,-0.0000188,0.072662,-0.0011841,0.0335953\Polar=86.6475392,-0.0634511,49.613327,-0.0625709,-0.0428135,142.5037566\PG=CS [SG(C8H6)]\NImag=0\0.10324752,-0.00000328,0.08416571,-0.00372843,0.00002162,1.41796485,-0.07762846,0.00001823,0.00037911,0.63429317,0.00003041,-0.06096032,0.00002887,-0.00004427,0.14976044,0.00042463,-0.00006522,-0.29489833,-0.00016210,0.00007155,0.67726032,-0.02730399,-0.00001580,0.00312398,0.00598322,0.00002108,0.00001557,0.04192830,-0.00001987,-0.03363500,-0.00004942,0.00000933,0.00682911,0.00004289,0.00000685,0.04013447,0.0321707,0.00007653,-1.06176800,-0.00004687,-0.00017297,-0.02108155,-0.00392273,0.00001853,1.49961283,-0.00023005,0.00000027,0.00007805,0.00649426,-0.00000210,0.00000660,-0.01946033,0.00000127,0.000081884,0.01327236,-0.00000311,-0.00071892,-0.00000200,0.00000481,0.00571363,-0.00001150,-0.00000241,-0.01560808,0.00002374,-0.00000003,0.01104704,-0.00001956,-0.00003784,0.00404803,0.00011017,0.00007620,0.00016044,0.00080054,-0.00000471,-0.41924786,-0.00090428,-0.00001016,0.41492874,0.00531250,0.00000211,0.01802335,-0.26644172,-0.00001405,0.10144697,-0.00134239,0.00000490,-0.00938341,-0.00019747,0.00000326,0.00028667,0.70500706,0.

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66,-0.00000019,-0.00000094,0.13267873,-0.00008793,-0.00000609,-0.00273
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.00001052,-0.00000397,-0.00005598,-0.00304596,0.00000734,-0.00147985,-
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123398,-0.00000755,0.13593061\\-0.00005282,0.,-0.00008719,-0.00000657,
0.,-0.00028801,0.00006824,0.,0.00025201,-0.00002570,0.,-0.00010842,0.0
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426,0.00000167,0.,-0.00009717,-0.00000554,0.,0.00023563,-0.00002481,0.
,-0.00004967,-0.00002688,0.,0.00000192,-0.00000034,0.,0.00000152,0.000
02592,0.,0.00000307,0.00002284,0.,-0.00005246\\\\@

Compound a18: optimisation archive

I\1\GINC-QUIMBY\FOpt\RB3LYP\6-31+G(d)\C8H5N1O2\GUY\22-Aug-2001\0\#B3LYP/6-31+G* OPT\1_nitrophenyl #B3LYP/6-31+g* optimization\0,1\,C,0.0046355363,0.,-3.2051136048\,C,0.0022647257,0.,-1.7765432482\,C,0.0076966749,0.,-4.4167210868\,H,0.0097141358,0.,-5.4845066454\,C,-1.2154444143,0.,-1.0652431455\,C,-1.2212344866,0.,0.3253949044\,C,-0.0015381271,0.,1.0039417261\,C,1.2200418497,0.,0.3287534206\,C,1.2180325553,0.,-1.0618672495\,H,-2.1524532538,0.,-1.6127114095\,H,-2.1487483088,0.,0.8854391036\,N,-0.0036656689,0.,2.4762198494\,H,2.1460240692,0.,0.8913257882\,H,2.156478876,0.,-1.6068680536\,O,1.0860953255,0.,3.0514758221\,O,-1.0951055403,0.,3.0482956745\Version=x86-Linux-G98RevA.7\State=1-A\HF=-512.9176402\RMSD=2.595e-09\RMSF=4.121e-05\Dipole=0.0016631,0.,-1.9146975\PG=CS [SG(C8H5N1O2)]\@

Compound a18: frequency calculation archive

I\1\GINC-CLUSTER18\Freq\RB3LYP\6-31+G(d)\C8H5N1O2\GUY\10-Jul-2002\0\#B3LYP/6-31+G* FREQ=NORAMAN GEOM=CHECKPOINT\1_nitrophenyl\0,1\,C,0.0046355363,0.,-3.2051136048\,C,0.0022647257,0.,-1.7765432482\,C,0.0076966749,0.,-4.4167210868\,H,0.0097141358,0.,-5.4845066454\,C,-1.2154444143,0.,-1.0652431455\,C,-1.2212344866,0.,0.3253949044\,C,-0.0015381271,0.,1.0039417261\,C,1.2200418497,0.,0.3287534206\,C,1.2180325553,0.,-1.0618672495\,H,-2.1524532538,0.,-1.6127114095\,H,-2.1487483088,0.,0.8854391036\,N,-0.0036656689,0.,2.4762198494\,H,2.1460240692,0.,0.8913257882\,H,2.156478876,0.,-1.6068680536\,O,1.0860953255,0.,3.0514758221\,O,-1.0951055403,0.,3.0482956745\Version=x86-Linux-G98RevA.7\State=1-A\HF=-512.9176402\RMSD=9.616e-09\RMSF=4.121e-05\Dipole=0.0016631,0.,-1.9146975\DipoleDeriv=-0.1256827,0.0087805,0.0081805,-0.0017435,-0.0350328,0.004641,0.0112652,-0.0117747,-0.1371921,0.1893573,-0.0068195,-0.011126,-0.0043384,0.0389208,-0.0058299,-0.0382407,0.0055481,0.6206156,-0.2251911,-0.001255,-0.0081473,0.0078153,-0.2603823,-0.0079804,0.0917588,-0.0204874,-0.4614378,0.2358355,-0.0005005,-0.0027175,-0.0011642,0.245106,0.0020743,-0.03545,0.010179,0.2672323,0.0188007,0.0056191,0.2150351,0.0010788,-0.1065777,-0.0019313,0.1765628,0.0128636,-0.2822525,-0.0327884,-0.008232,0.144398,0.0047225,-0.0663442,-0.0088051,-0.1733453,0.0093527,0.2637353,0.1105493,-0.0063381,-0.015256,-0.0049558,0.0477451,0.0054564,0.0115026,-0.0074449,-0.8340316,-0.0616712,0.0109797,-0.129441,0.0027992,-0.0619672,-0.0044788,0.1529486,-0.0034372,0.2150135,0.0181948,0.003701,-0.1959048,-0.00331,-0.1083499,0.0068229,-0.2148181,0.0107194,-0.2778279,0.0014737,-0.003953,-0.0647056,-0.0021707,0.1372657,0.0056435,-0.0490814,-0.0035794,0.0203933,0.0487853,0.0047314,0.0276596,-0.0016778,0.1449491,0.0047096,0.0411095,-0.0029248,0.0948897,1.5535497,-0.0112841,-0.0571673,0.006835,0.2260919,-0.0047586,0.001809,0.00398,2.3291917,0.0687639,-0.002588,-0.0205237,0.0004024,0.1438841,-0.0009061,-0.0306215,-0.0006588,0.0994268,0.0074556,-0.0033039,0.0616962,-0.0005045,0.1366628,0.0014001,0.0514718,0.0002807,0.0224065,-0.8992626,0.0022361,-0.3624797,-0.0014396,-0.2409715,0.0017434,-0.355037,0.0022806,-0.9558894,-0.9081763,0.0082351,0.4105393,-0.0023496,-0.2409993,0.0022035,0.3581465,-0.0048775,-0.9841856\Polar=101.9956869,0.5423554,53.3374625,1.96179,-0.9338048,189.2476275\PG=CS [SG(C8H5N1O2)]\NImag=0\0.10277927,-0.00000433,0.08760199,-0.00399655,-0.00007543,1.42451401,-0.07769248,0.0000980,0.00100591,0.63181203,-0.00015705,-0.06552271,-0.00029525,0.00008196,0.15485326,-0.00206627,-0.00001944,-0.30052848,0.00115935,-0.00051632,0.67458818,-0.02778316,-0.00000173,0.00249108,0.00594323,-0.00004394,-0.00028538,0.04292800,0.00000506,-0.03631916,0.00028004,0.00000616,0.00750938,0.00013982,0.00002406,0.04454971,0.00676312,0.00000902,-1.06079667,-0.00217952,0.00103286,-0.01060734,-0.00268958,-0.00015039,1.48342074,0.00001531,-0.00000263,0.00003385,0.00648995,-0.00001023,-0.00009352,-0.01998150,0.00000997,0.00092856,0.01351224,-0.00002454,0.000

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