

Electronic Supplementary Information for

Recent Advances in the Chemistry of Benzo[e][1,2,4]triazinyl Radicals

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Table of Contents

Appendix 1. Experimental Details	S2
General Experimental.....	S2
Synthesis of 3- <i>tert</i> -butyl Analogue 10	S2
CW-EPR and Simulation	S2
Appendix 2. Computational Spectroscopy	S3
Computational Methods	S3
Calculation of Natural Transition Orbitals of 10	S3
Gaussian Archive Entries	S4
Appendix 3. Swain-Lupton Correlations.....	S7
Analysis	S7
Gaussian Archive Entries	S10
References	S35

Appendix 1. Experimental Details

Experiments were performed to generate Figures 9, 11 and 16 as follows.

General Experimental

UV-visible spectra were measured using a Cary 60 spectrophotometer, analysing a 1 mM solution of **10** in dichloromethane in a quartz cuvette, at ambient temperature. All solvents were dried over activated 4Å molecular sieves prior to analysis. IR was measured in the solid phase on a Bruker Alpha II FT-IR spectrometer at room temperature. Mass spectrometry was performed with a Waters LC Premier™ XE oa-TOF spectrometer. Electrochemical experiments were carried out using a PalmSens4 Potentiostat/Galvanostat/Impedance Analyzer and a single compartment three-electrode glass cell. Electrochemical experiments were performed at room temperature (23 ± 2 °C) under argon. Glassy carbon disks (0.065 cm²) served as the working electrode, a platinum coil was used as counter electrode, and silver/silver chloride as the reference electrode. 5 mg of **10** (2 mM) was dissolved in 1.0×10^{-1} M MeCN/Bu₄NClO₄. The solution was stirred and bubbled briefly under argon prior to measurement. All cyclic voltammograms were obtained after bubbling, with no stirring. The cell iR drop was not compensated during measurement. CW-X-Band EPR spectra were measured on a commercial Bruker E500 spectrometer equipped with a Bruker ER4122 SHQE resonator. Samples were loaded into conventional X-Band EPR tubes with an inner diameter of 2.8 mm. Spectra were measured at room temperature using 47 uW, 9.8 GHz microwaves and 0.1 G modulation amplitude. The sample was dissolved in toluene and degassed with Ar prior to the taking of measurements, also performed at room temperature.

Synthesis of 3-*tert*-butyl Analogue **10**

N,N'-Diphenylbenzohydrazonamide **10a** was prepared as per literature methods.^{1,2}

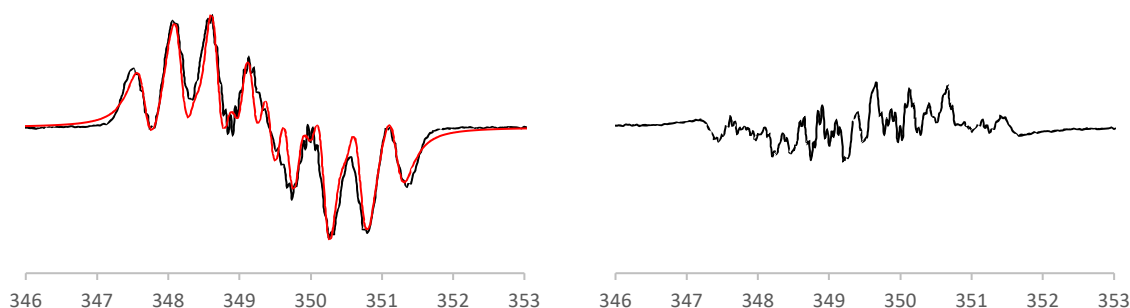
Following the procedure described by Koutentis *et al.*³ (Scheme 8), **10a** (401 mg, 1.5 mmol) was added to 1,8-diazabicyclo[5.4.0]undec-7-ene (0.22 mL, 1.5 mmol) in dichloromethane (15 mL). Pd/C (1.6 mol%) was added to the solution which was stirred open to the air for 6 h. Radical **10** was purified by column chromatography on basic alumina (eluting with 1:3 dichloromethane to hexane) to give 316 mg (1.19 mmol 79%) as red prismatic crystals.

IR (solid, ATR): 2957, 1580, 1493, 1479, 1453, 1399, 1188, 840, 779, 760, 748, 698 cm⁻¹.

TOF MS ES+: *m/z* (%) = 264 (100) [M⁺], 265 (72) [(M + H)⁺], 266 (23).

UV-Vis (CH₂Cl₂): λ_{max} (log ϵ) = 243 (3.48), 322 (3.02), 350 (2.99), 430 (2.78).

CW-EPR and Simulation



(Left) Experimental cw-EPR spectrum (Black) and simulated spectrum (Red) assuming hyperfine coupling constants of 7.4 G (N1), 5.1 G (N2,4) and a g factor of 2.004. Artificial line broadening imposed as H couplings were not resolved. (Right) Difference spectra. Field strength given in mT.

Appendix 2. Computational Spectroscopy

Computational chemistry was undertaken to analyse the spectrum in Figure 9.

Computational Methods

All calculations were performed in the Gaussian 16 Rev. C.01 quantum chemistry package.⁴ Geometries were optimised at the M06-2X/6-31+G(d,p) level of theory for reduction potentials,⁵⁻⁷ and the B3LYP and M06-2X/6-311+G(d,p) level of theory for TD-DFT and *natural transition orbital* (NTO) calculations.^{8, 9} The effect of dichloromethane was modelled with the SMD solvation method as implemented in Gaussian.¹⁰ All structures were confirmed as local minima by vibrational analysis (*i.e.* possessing no imaginary frequencies). For reduction potentials, Gibbs free energies in solution (G_{soln}°) were then determined from the ideal gas molecular partition functions at 298.15 K, assuming the *rigid rotor harmonic oscillator* (RRHO) formalism and appropriate frequency scaling factors. Absolute reduction potentials were thus determined via the “direct method” in conjunction with EC-FD convention for the electron, as described by Ho *et al.*¹¹ Output from all calculations performed in this work are given as Gaussian archive entries in S4 and S11.

Calculation of Natural Transition Orbitals of **10**

Although M06-2X identified one major absorption in the UV region, B3LYP is more accurate in terms of cm^{-1} and was selected for NTO visualisation. Nevertheless, based on the major absorption predicted by the M06-2X functional, absorption 27 in B3LYP was identified as the chief feature in the UV/Vis spectra of **10**.

TD-DFT output for select absorptions.

M062X

```
Excited State 1: 2.085-A      2.7258 eV  454.86 nm  f=0.0039  <S**2>=0.837
  71A -> 72A      0.78505
  71A -> 73A      0.40675
  71A -> 74A     -0.34547
  71A -> 75A      0.11882

Excited State 24: 2.520-A      5.5289 eV  224.25 nm  f=0.2799  <S**2>=1.338
  67A -> 72A     -0.27480
  67A -> 73A     -0.17000
  67A -> 74A      0.15055
  68A -> 72A      0.11475
  70A -> 72A      0.47107
  70A -> 73A      0.10227
  70A -> 74A     -0.12147
  71A -> 83A      0.11299
  62B -> 71B      0.13688
  64B -> 71B      0.28289
  67B -> 71B     -0.13611
  67B -> 72B     -0.23743
  68B -> 74B      0.10214
  70B -> 72B      0.41836
  70B -> 74B     -0.11110

Excited State 26: 2.356-A      5.5800 eV  222.20 nm  f=0.1095  <S**2>=1.138
  66A -> 72A      0.13715
  67A -> 72A      0.13994
  67A -> 73A      0.12834
  67A -> 74A     -0.10373
  68A -> 72A      0.14991
  70A -> 72A     -0.24531
  70A -> 73A     -0.10380
  71A -> 77A      0.10460
  71A -> 79A     -0.17124
  71A -> 80A     -0.15182
```

71A -> 81A	0.18819
71A -> 82A	0.10896
71A -> 83A	-0.13160
71A -> 84A	0.18055
71A -> 86A	0.17815
62B -> 71B	0.27833
64B -> 71B	0.41720
66B -> 72B	0.13680
67B -> 72B	-0.33184
67B -> 74B	0.14373
70B -> 71B	-0.13482
70B -> 72B	-0.16817

B3LYP

Excited State 1: 2.085-A 2.5182 eV 492.35 nm f=0.0054 <S**2>=0.837

71A -> 72A	0.92721
71A -> 73A	-0.19000
71A -> 74A	-0.22554
66B -> 71B	-0.10276

Excited State 27: 2.135-A 5.1549 eV 240.52 nm f=0.2133 <S**2>=0.890

67A -> 72A	-0.12788
68A -> 72A	0.13559
68A -> 73A	-0.11662
69A -> 72A	0.32487
69A -> 74A	-0.10242
70A -> 72A	0.48647
70A -> 73A	0.25303
71A -> 82A	0.20342
64B -> 71B	-0.10061
66B -> 71B	0.10966
66B -> 73B	0.14799
69B -> 72B	0.23203
70B -> 72B	-0.47975
70B -> 73B	-0.22364

Excited State 32: 2.315-A 5.3754 eV 230.65 nm f=0.2562 <S**2>=1.089

66A -> 72A	-0.12396
67A -> 72A	0.11613
68A -> 72A	0.11757
69A -> 72A	0.12009
69A -> 73A	-0.20509
70A -> 72A	0.24597
70A -> 73A	-0.29707
70A -> 74A	-0.17364
71A -> 84A	0.27626
62B -> 71B	-0.11093
64B -> 71B	0.42719
66B -> 72B	0.16540
67B -> 72B	0.16460
68B -> 72B	0.10955
69B -> 73B	-0.19266
70B -> 72B	-0.14541
70B -> 73B	0.30790
70B -> 74B	-0.30270
70B -> 75B	0.16164

Gaussian Archive Entries

B3LYP TD-DFT

H-tBu-Tri.nd.B3LYP.dichloromethane.TD

```
1\1\GINC-GADI-CPU-CLX-2142\SP\UB3LYP TD-FC\6-311+G(d,p)\C17H18N3(2)\FJ
R502\21-May-2020\0\#\ B3LYP/6-311+G** SCF=XQC IOP(2/17=4) INT(grid=ult
rafine) SCRF=(SMD,Solvent=dichloromethane) TD(Nstates=40) maxdisk=50GB
\\H-tBu-Tri.nd.B3LYP.dichloromethane.TD\0,2\N,0,-2.8651304864,1.66930
16118,0.0263708518\C,0,-2.8697452953,0.3403533263,0.0526613631\N,0,-3.
9480097147,-0.4492329415,0.0154141086\C,0,-5.1609668088,0.1698767304,-
```

0.1359385683\C,0,-5.2681568827,1.5877937495,-0.1966440775\N,0,-4.0799079914,2.2933276346,-0.0434002359\C,0,-6.5120356881,2.1960052874,-0.4235755665\C,0,-7.6485099731,1.4075775069,-0.5484733678\C,0,-7.5636965535,0.0105573435,-0.456064707\C,0,-6.3352514145,-0.5983083292,-0.2577144134\C,0,-1.5028688676,-0.3530449394,0.1510605286\H,0,-6.58764294,3.2717584284,-0.5038310434\H,0,-8.607100726,1.8827067445,-0.7224938482\H,0,-8.4591424177,-0.5930784177,-0.5502449898\H,0,-6.2431226564,-1.6769869611,-0.2017731679\C,0,-4.0088248919,3.7254237826,-0.0014711596\C,0,-4.6901226816,4.4323694078,0.9907539288\H,0,-5.2820508311,3.9009755597,1.7262016176\C,0,-4.5879416875,5.8214893742,1.0346674273\H,0,-5.1120201219,6.3709428081,1.8084762056\C,0,-3.8050019434,6.4995761943,0.1001703893\H,0,-3.7258832441,7.5801113141,0.1397343828\C,0,-3.1194208178,5.7835698939,-0.8819087745\H,0,-2.5083526734,6.305049872,-1.6099545724\C,0,-3.218486757,4.3952813924,-0.9367791322\H,0,-2.6896811873,3.8302918057,-1.6945018043\C,0,-0.3417077855,0.6539890979,0.1726775886\C,0,-1.3366152627,-1.2905846427,-1.0650900062\C,0,-1.470563635,-1.1904620741,1.4487707991\H,0,-0.3156832585,1.2624982099,-0.7345445331\H,0,0.6041402457,0.1084201966,0.241895424\H,0,-0.406695901,1.3305831754,1.0279362012\H,0,-1.3471635668,-0.7271401649,-2.0034700904\H,0,-2.1348044137,-2.0345022126,-1.1042662498\H,0,-0.3792426762,-1.8163403827,-0.9990533934\H,0,-1.5776248988,-0.5538409367,2.3326236486\H,0,-0.5138902619,-1.7159996393,1.526084868\H,0,-2.2714633319,-1.9324688058,1.4622943686\\Version=ES64L-G16RevC.01\State=2-A\HF=-823.1065159\S2=0.763027\S2-1=0.\S2A=0.750109\RMSD=4.229e-09\PG=C01 [X(C17H18N3)]\@

B3LYP Optimisation

H-tBu-Tri.nd.B3LYP.dichloromethane

1\1\GINC-GADI-CPU-CLX-2142\FOpt\UB3LYP\6-311+G(d,p)\C17H18N3(2)\FJR502\20-May-2020\0\#\ B3LYP/6-311+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-tBu-Tri.nd.B3LYP.dichloromethane\0,2\N,-2.8651304864,1.6693016118,0.0263708518\C,-2.8697452953,0.3403533263,0.0526613631\N,-3.9480097147,-0.4492329415,0.0154141086\C,-5.1609668088,0.1698767304,-0.1359385683\C,-5.2681568827,1.5877937495,-0.1966440775\N,-4.0799079914,2.2933276346,-0.0434002359\C,-6.5120356881,2.1960052874,-0.4235755665\C,-7.6485099731,1.4075775069,-0.5484733678\C,-7.5636965535,0.0105573435,-0.456064707\C,-6.3352514145,-0.5983083292,-0.2577144134\C,-1.5028688676,-0.3530449394,0.1510605286\H,-6.58764294,3.2717584284,-0.5038310434\H,-8.607100726,1.8827067445,-0.7224938482\H,-8.4591424177,-0.5930784177,-0.5502449898\H,-6.2431226564,-1.6769869611,-0.2017731679\C,-4.0088248919,3.7254237826,-0.0014711596\C,-4.6901226816,4.4323694078,0.9907539288\H,-5.2820508311,3.9009755597,1.7262016176\C,-4.5879416875,5.8214893742,1.0346674273\H,-5.1120201219,6.3709428081,1.8084762056\C,-3.8050019434,6.4995761943,0.1001703893\H,-3.7258832441,7.5801113141,0.1397343828\C,-3.1194208178,5.7835698939,-0.8819087745\H,-2.5083526734,6.305049872,-1.6099545724\C,-3.218486757,4.3952813924,-0.9367791322\H,-2.6896811873,3.8302918057,-1.6945018043\C,-0.3417077855,0.6539890979,0.1726775886\C,-1.3366152627,-1.2905846427,-1.0650900062\C,-1.470563635,-1.1904620741,1.4487707991\H,-0.3156832585,1.2624982099,-0.7345445331\H,0.6041402457,0.1084201966,0.241895424\H,-0.406695901,1.3305831754,1.0279362012\H,-1.3471635668,-0.7271401649,-2.0034700904\H,-2.1348044137,-2.0345022126,-1.1042662498\H,-0.3792426762,-1.8163403827,-0.9990533934\H,-1.5776248988,-0.5538409367,2.3326236486\H,-0.5138902619,-1.7159996393,1.526084868\H,-2.2714633319,-1.9324688058,1.4622943686\\Version=ES64L-G16RevC.01\State=2-A\HF=-823.1065159\S2=0.763027\S2-1=0.\S2A=0.750109\RMSD=2.491e-09\RMSF=9.105e-06\Dipole=-0.7697903,1.4435472,-0.1117303\Quadrupole=2.2669833,2.6602648,-4.9272481,-1.3484392,-2.3140723,0.4157309\PG=C01 [X(C17H18N3)]\@

M06-2X TD-DFT

H-tBu-Tri.nd.M062X.dichloromethane.TD

1\1\GINC-GADI-CPU-CLX-0859\SP\UM062X TD-FC\6-311+G(d,p)\C17H18N3(2)\FJR502\22-May-2020\0\#\ M062X/6-311+G** SCF=XQC IOP(2/17=4) INT(grid=ult

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```

M06-2X Optimisation

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ne) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\\H-tBu-Tri.nd.
M062X.dichloromethane\\0,2\\N,-2.8628538098,1.6680805344,0.0068885018\\C
,-2.869999211,0.3422635675,0.0506550948\\N,-3.9439376089,-0.4458359873,
0.0462884587\\C,-5.153239295,0.1755954374,-0.1063104046\\C,-5.2554471577
,1.5860795733,-0.1886911908\\N,-4.0678963221,2.2875333178,-0.0455167006
\\C,-6.4941213731,2.1973472705,-0.4314890063\\C,-7.6289140383,1.41315995
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415\\H,-6.5623919508,3.2713826919,-0.5400126819\\H,-8.5847791577,1.88752
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2624328514,6.3535558781,1.7005045163\\C,-3.8083246912,6.478490547,0.118
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\\Dipole=-0.7914752,1.4380836,-0.127145\\Quadrupole=3.3574573,3.0320387,
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```

Appendix 3. Swain-Lupton Correlations

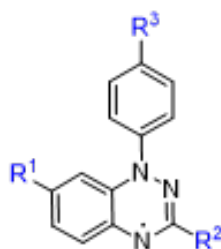
Detailed here is the analysis of electrochemical data, given in the main text.

Analysis

The modelling given here is illustrative and by no means an exhaustive take on the concept. Gibbs free energies in solution G°_{soln} are given in hartrees whilst $E_{1/2}$ are given in volts, based on the expression

$$E_{1/2} = 27.2114(G^{\circ}_{soln}(Ox) - G^{\circ}_{soln}(Red) + G^{\circ}_{gas}(e^{-}))$$

where “Red” is the reduced species, “Ox” is the oxidised species and $G^{\circ}_{gas}(e^{-})$ is -3.632 (in kJ mol⁻¹) at 298.15 K assuming the EC-FD convention.



$R^1 = \text{H, Me, OMe, NO}_2, \text{CF}_3, \text{Cl}$

$R^2 = \text{Ph, CF}_3, 4\text{-(Me, OMe, NO}_2, \text{Cl)-C}_6\text{H}_4$

$R^3 = \text{H, Me, OMe, NO}_2, \text{CF}_3, \text{Cl}$

Radicals considered in the modelling.

C7	C3	N1 (Ar para)	G°_{soln} Radical	G°_{soln} Cation	G°_{soln} Anion	$E_{1/2}^{0/+1}$	$E_{1/2}^{-1/0}$
H	Ph	H	-896.14715	-895.97139	-896.2682	4.74	3.26
Me	Ph	H	-935.42479	-935.25163	-935.54291	4.67	3.18
H	PhMe	H	-935.42467	-935.24995	-935.545	4.72	3.24
H	Ph	Me	-935.42405	-935.24896	-935.54336	4.73	3.21
MeO	Ph	H	-1010.6036	-1010.434	-1010.7215	4.58	3.17
H	PhOMe	H	-1010.604	-1010.4301	-1010.7247	4.69	3.25
H	Ph	MeO	-1010.6031	-1010.4292	-1010.7212	4.69	3.18
Cl	Ph	H	-1355.727	-1355.5467	-1355.8517	4.87	3.36
H	PhCl	H	-1355.7296	-1355.5522	-1355.8515	4.79	3.28
H	Ph	Cl	-1355.7276	-1355.5498	-1355.8516	4.80	3.34
NO2	Ph	H	-1100.5845	-1100.3952	-1100.7217	5.11	3.69
H	PhNO2	H	-1100.5853	-1100.4065	-1100.7105	4.83	3.37
H	Ph	NO2	-1100.5837	-1100.402	-1100.7198	4.91	3.67
CF3	Ph	H	-1233.1028	-1232.9179	-1233.2319	4.99	3.48
H	CF3	H	-1002.1862	-1001.9977	-1002.3166	5.09	3.51
H	Ph	CF3	-1233.1028	-1232.9238	-1233.2319	4.83	3.48

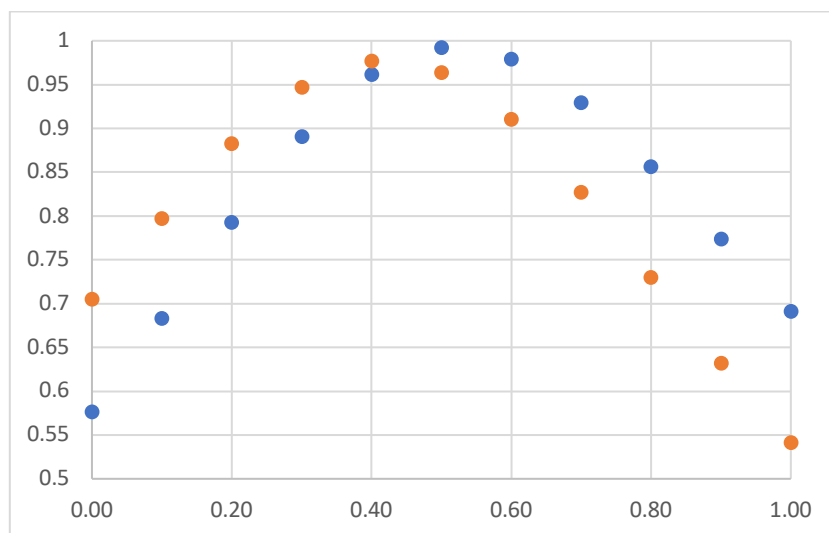
Modified Swain-Lupton resonance and field-inductive parameters (R and F) taken from Hansch *et al.*¹²

Substituent	R	F
H	0	0.03
Ph	-0.13	0.12
Me	-0.18	0.01
PhMe	-0.15	0.12
Cl	-0.19	0.42
PhCl	-0.06	0.18
NO2	0.13	0.65

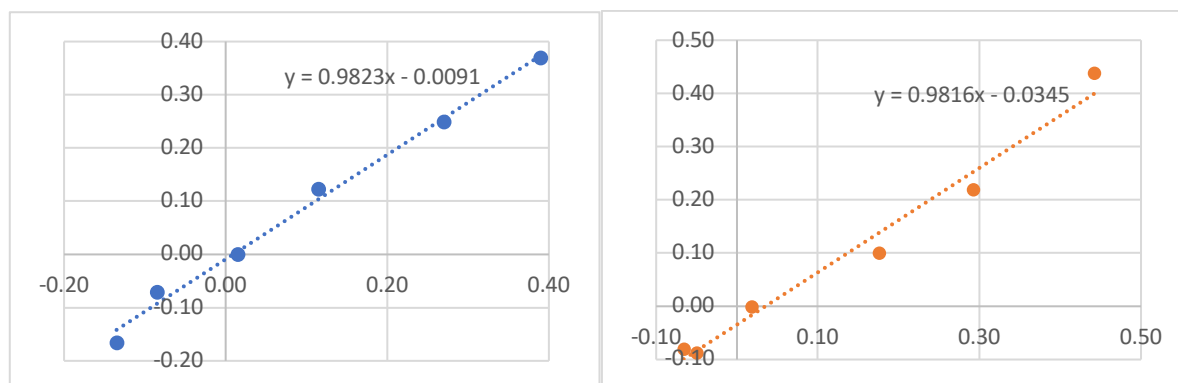
PhNO2	0	0.26
CF3	0.16	0.38
OMe	-0.56	0.29
PhOMe	-0.21	0.13

C7 position

Scan of the ratio formula $xR + (1 - x)F$ between $x = 0$ and $x = 1$ at 0.1 increments, where the y-axis is the correlation measure (R^2) of the linear regression model. Blue dots represent oxidation and orange dots represent reduction.

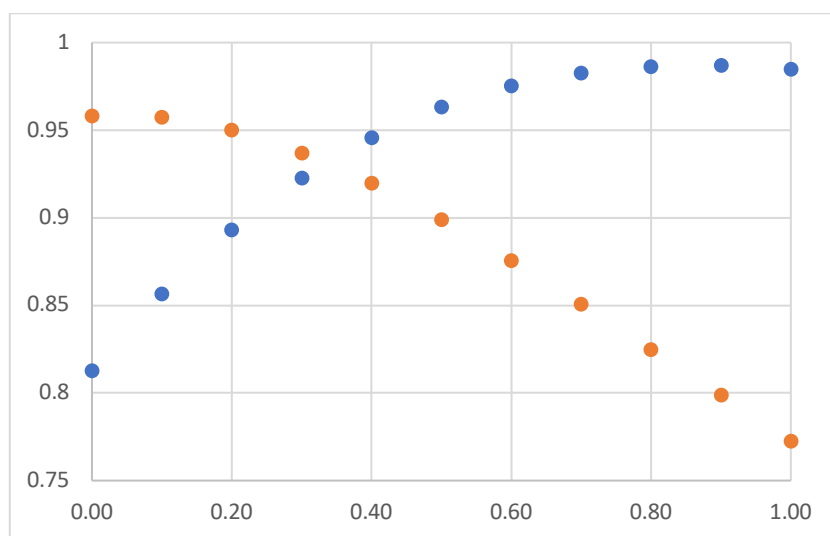


Swain-Lupton expression (x-axis) against $E_{1/2}$ (y-axis) for the best fit (*vide supra*). (Left) Oxidation assuming the expression $\frac{1}{2}(R + F)$. (Right) Reduction assuming the expression $0.4R + 0.6F$.

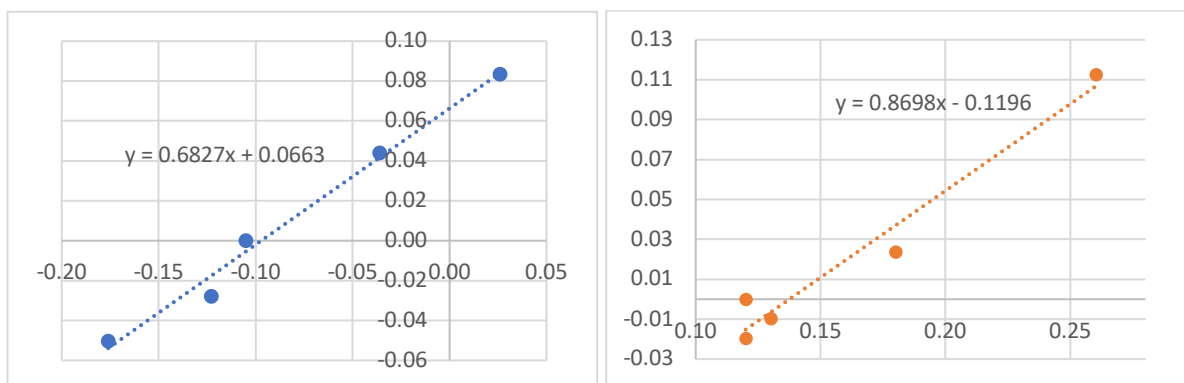


C3 position

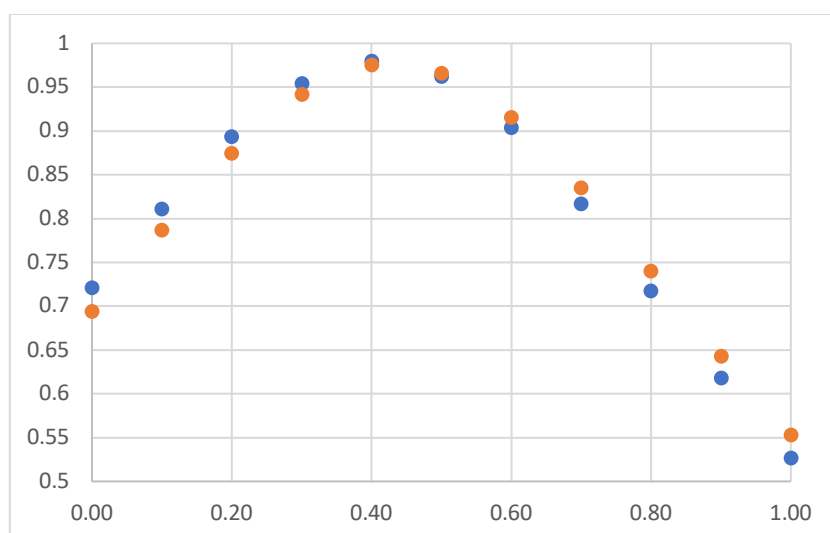
Unlike the C7 and N1 positions, far better correlations were found in treating the C3 substituent in its entirety (*e.g.* by treating the MeO group as an anisole substituent). Although a CF₃ group was also included in the modelling, the resultant fit was poor, so it was discarded. Here, the isodesmic method (in combination with a modest level of theory) is likely breaking down given that the group is non-aryl. Indeed, the reduction potentials predicted relative to Blatter's radical were considerably higher (> 200 mV) than experimentally measured, unlike other radicals modelled here.¹³



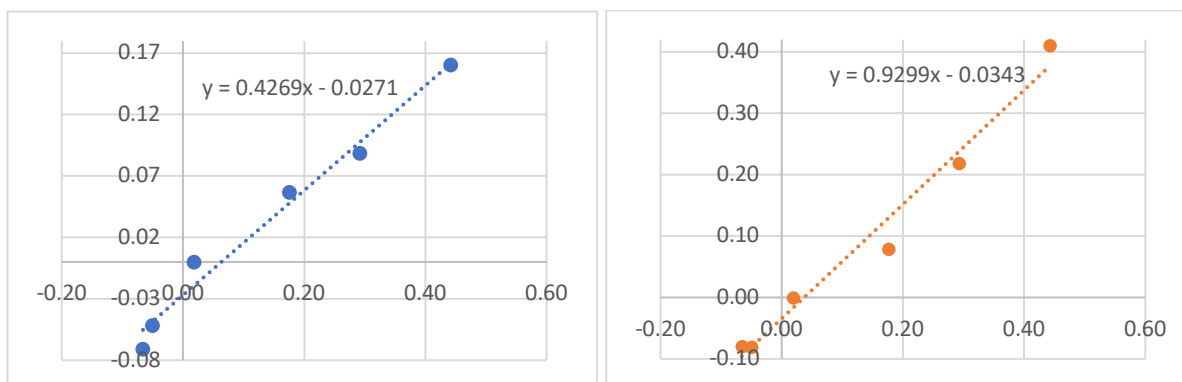
Swain-Lupton expression (x-axis) against $E_{1/2}$ (y-axis) for the best fit (*vide supra*). (Left) Oxidation assuming the expression $0.9R + 0.1F$. (Right) Reduction assuming the expression $0R + 1F$. Better fits were produced by discarding the CF_3 data point, shown here.



N1 aromatic position (*para* position)



Swain-Lupton expression (x-axis) against $E_{1/2}$ (y-axis) for the best fit (*vide supra*). (Left) Oxidation assuming the expression $0.4R + 0.6F$, same fit for reduction (Right).



Gaussian Archive Entries

Where “nd” is the radical, “cs” is the cation and “as” is the anion.

7-trifluoromethyl radical

CF3-Ph-Ph.as

```
1\1\GINC-GADI-CPU-CLX-0787\FOpt\RM062X\6-31+G(d,p)\C20H13F3N3(1-)\FJR5
02\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultraf
ine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\CF3-Ph-Ph.as
\ -1,1\C, -3.5912056469,1.2384615257,-0.6471348676\C, -3.6019377275,-0.0
992100079,-0.2700484816\C, -2.4165140502,-0.7052699091,0.1470404528\C, -
1.215397188,0.0169477506,0.2298546399\C, -1.2537572348,1.4099030088,-0.
0726980471\C, -2.4067661242,1.9951161156,-0.5678643466\N, -0.0408764203,
2.0829962634,0.1809953528\N, -0.0309645571,-0.6027029655,0.5414423684\C
,1.0652247989,0.1009734102,0.1779583352\N,1.1443123636,1.3715108939,-0
.1322170767\C,0.0895804458,3.4666532636,0.2617779037\C,-0.9085832507,4
.2486132621,0.8809403248\H,-1.7951753365,3.770860141,1.2847241336\C,-0
.7527194545,5.6232401872,1.004292426\H,-1.5349366391,6.198820661,1.491
7274691\C,0.3959008555,6.2641821337,0.5283136012\C,1.3916483143,5.4922
493325,-0.0669313552\H,2.2965217492,5.9658270736,-0.4386002354\C,1.251
2237643,4.1112791266,-0.2022326349\H,2.0331986213,3.5214513417,-0.6627
87533\H,-4.5210932742,-0.6745867349,-0.3122568121\H,-2.3988300992,-1.7
587585037,0.410351498\H,-2.4154092869,3.0427598648,-0.8526672089\H,0.5
11504123,7.3386472905,0.6289430158\C,2.3488930325,-0.6655337561,0.0617
501644\C,2.3326393274,-2.0637908829,0.0157931751\H,1.3778771634,-2.576
2638311,0.0633229139\C,3.522711705,-2.7836435366,-0.0914651033\H,3.493
787101,-3.8689007756,-0.129046881\C,4.7448951644,-2.1146778229,-0.1529
903832\C,4.7695593149,-0.7191885481,-0.1018554229\H,5.7173451231,-0.18
99015193,-0.1410611941\C,3.5814528324,-0.0007424684,0.0079644348\H,3.5
984682729,1.083054444,0.0598157051\H,5.6717866154,-2.6749004759,-0.236
1570863\C,-4.8271581801,1.9223166553,-1.1139730376\F,-5.8911832035,1.0
996573074,-1.1953425395\F,-5.2036338334,2.9464467046,-0.3048623622\F,-
4.6860391812,2.4827539801,-2.3414953054\Version=ES64L-G16RevC.01\Stat
e=1-A\HF=-1233.4581859\RMSD=6.710e-09\RMSF=3.965e-06\Dipole=0.5113374,
0.6154492,-0.1582129\Quadrupole=-6.6033335,6.0548471,0.5484864,4.71710
52,-7.4400866,3.3562444\PG=C01 [X(C20H13F3N3)]\@
```

CF3-Ph-Ph.cs

```
1\1\GINC-GADI-CPU-CLX-1645\FOpt\RM062X\6-31+G(d,p)\C20H13F3N3(1+)\FJR5
02\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultraf
ine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\CF3-Ph-Ph.cs
\ 1,1\C, -3.5944350806,1.3548032103,-0.5719198602\C, -3.6076621327,-0.06
90684206,-0.5168550468\C, -2.4449349244,-0.7613472219,-0.3336974205\C, -
1.221462509,-0.051848043,-0.1861483523\C, -1.2445479192,1.3774071332,-0
.1950732582\C, -2.4488540897,2.0869621534,-0.417922256\N, -0.0397006085,
1.9838150915,0.0050799775\N, -0.0696462224,-0.7181712564,-0.0613670951\C
,1.0469806951,-0.0125507315,0.0372454715\N,1.0763936024,1.3423752361,
0.1013470196\C,0.0859223746,3.4275517317,0.1217790427\C,-0.6302033313,
```

4.087788793,1.1153629787\H,-1.2823460093,3.5386509761,1.7877578899\C,-0.4595093418,5.4641858131,1.2362775912\H,-0.9969402798,6.0020410846,2.0099044094\C,0.4036165245,6.1427196304,0.3750072255\C,1.1129074371,5.4515774417,-0.608709567\H,1.7838609862,5.9829707252,-1.2750156696\C,0.9656875852,4.0737765458,-0.7398934251\H,1.508565873,3.5112933479,-1.4929882905\H,-4.546507969,-0.5978756096,-0.6395564725\H,-2.4143493574,-1.8448366347,-0.3102625927\H,-2.4587202096,3.1697440033,-0.4777647471\H,0.5280307002,7.2160781632,0.4744958307\C,2.352026739,-0.6959699457,0.1107349347\C,2.4065042583,-2.0881852077,-0.0388039434\H,1.492749861,-2.6484622506,-0.2046570941\C,3.6319277089,-2.7429581325,0.0222362798\H,3.6722038772,-3.8208119049,-0.096800457\C,4.8048232704,-2.0162505118,0.2341505902\C,4.7511973642,-0.6299718373,0.3846010905\H,5.6618961651,-0.0639563577,0.5514930643\C,3.5300071463,0.0337284522,0.3228894834\H,3.4910243005,1.1109188871,0.4427771346\H,5.7599055559,-2.5302411356,0.281857597\C,-4.8789346245,2.1141708343,-0.8167213877\F,-5.9271772838,1.2988032067,-0.9768494249\F,-5.1629453565,2.9381045777,0.2068999967\F,-4.7910047756,2.8796881632,-1.9175712473\\Version=ES64L-G16RevC.01\State=1-A\HF=-1233.1477338\RMSD=8.094e-09\RMSF=8.863e-06\Dipole=0.879253,0.2694793,0.2528829\Quadrupole=2.0483804,16.5649539,-18.6133343,3.1514613,-2.4517988,3.5527229\PG=C01 [X(C20H13F3N3)]\@

CF3-Ph-Ph.nd

1\1\GINC-GADI-CPU-CLX-1646\FOpt\UM062X\6-31+G(d,p)\C20H13F3N3(2)\FJR502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\\CF3-Ph-Ph.nd\0,2\C,-3.6217504194,1.3291692594,-0.580460311\C,-3.623047631,-0.0705777603,-0.5389537931\C,-2.4301057482,-0.7447308432,-0.3467419811\C,-1.2235027278,-0.0418744638,-0.180137862\C,-1.2554291101,1.3779493696,-0.1856571192\C,-2.453424529,2.0623096346,-0.4108845225\N,-0.0387482691,2.0151436731,0.0172050931\N,-0.0492626464,-0.7283331488,-0.0399310275\C,1.0570384627,0.0087596118,0.0364319767\N,1.1274745604,1.3405140248,0.0667598418\C,0.0886352263,3.4370759143,0.1301700598\C,-0.6381265073,4.1221613269,1.1033525188\H,-1.3045617573,3.5798561248,1.7675972546\C,-0.4836049549,5.5021083058,1.2164019683\H,-1.0427735632,6.0422081573,1.9737571796\C,0.3944218022,6.1826334026,0.3720632822\C,1.1240042873,5.4816598887,-0.5891167692\H,1.8097112902,6.0081791211,-1.2453444182\C,0.9743286808,4.1025302073,-0.7157828212\H,1.5337194954,3.5397642389,-1.456331114\H,-4.5485748991,-0.6205398347,-0.6677722605\H,-2.3936944912,-1.8289936232,-0.3299012473\H,-2.4743784346,3.1458768243,-0.4563589076\H,0.5133209144,7.2573977627,0.4664083717\C,2.3667570756,-0.7002703789,0.1072284527\C,2.4100024669,-2.0928708492,-0.0271870609\H,1.486831583,-2.640868576,-0.1805265934\C,3.6279668235,-2.7665141625,0.0333184587\H,3.6503654078,-3.846743953,-0.0739988978\C,4.8132019209,-2.0574576174,0.2291762457\C,4.7744432467,-0.668860963,0.3645443067\H,5.6928993574,-0.1109152769,0.5195486713\C,3.5591594208,0.0082117137,0.304325631\H,3.5303015215,1.0869765959,0.4129071422\H,5.7620226022,-2.5834977982,0.2764511177\C,-4.8953984884,2.0902991143,-0.8022654857\F,-5.9499012984,1.2870388772,-1.015048958\F,-5.2097504164,2.8731875991,0.2530390357\F,-4.814220254,2.9186885008,-1.8649654583\\Version=ES64L-G16RevC.01\State=2-A\HF=-1233.3291975\S2=0.768289\S2-1=0.\S2A=0.750208\RMSD=8.478e-09\RMSF=4.642e-06\Dipole=0.7589072,0.8967073,0.176536\Quadrupole=-5.624829,12.4855961,-6.8607671,5.5080251,-4.2486619,3.024875\PG=C01 [X(C20H13F3N3)]\@

7-chloro radical

Cl-Ph-Ph.as

1\1\GINC-GADI-CPU-CLX-2393\FOpt\RM062X\6-31+G(d,p)\C19H13Cl1N3(1-)\FJR502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\\Cl-Ph-Ph.as\0,1\C,-3.5505185284,1.3418536471,-1.1039605999\C,-3.6669192621,-0.0028128649,-0.7917550458\C,-2.5599848211,-0.6639236963,-0.2493992886\C,-1.3613029046,0.0079583973,0.0207709699\C,-1.3115211985,1.4036855045,-0.2370763996\C,-2.3756945669,2.0564543758,-0.8519560557\N,-0.1123435013,2.0206273864,0.1709913695\N,-0.2420689995,-0.6695643887,0.4683936345

\C,0.9093517256,-0.0067104058,0.249795242\N,1.0747377516,1.2664967345,
-0.0332533487\C,0.0594990347,3.3900258456,0.3303681946\C,-0.9806792706
,4.1949800325,0.8439940611\H,-1.9318608514,3.7444292361,1.106832548\C,
-0.787439156,5.5553931445,1.0462980662\H,-1.6047083483,6.1471110701,1.
4498150376\C,0.4396216821,6.1613027578,0.7563503831\C,1.4746041084,5.3
666116181,0.2670773441\H,2.4400627702,5.8115569543,0.0406805537\C,1.29
89231892,3.9996259141,0.0548557788\H,2.1118465191,3.3931599103,-0.3223
364762\H,-4.5944640224,-0.5348437241,-0.9766682669\H,-2.6146441385,-1.
726408739,-0.0294070263\H,-2.3162772824,3.110139133,-1.1003766034\C,2.
1716255764,-0.8171789923,0.27426035\C,2.1188606613,-2.2069563265,0.121
9357267\H,1.1524201185,-2.6794821106,-0.0171883252\C,3.2872096271,-2.9
68346459,0.1433017603\H,3.2303575799,-4.0461653559,0.0202504866\C,4.52
4908672,-2.349366526,0.3185990389\C,4.5856167271,-0.9632394574,0.47621
3832\H,5.5445325123,-0.4738201421,0.621154846\C,3.417897913,-0.2034356
829,0.4570218415\H,3.4612757055,0.8727271451,0.5909953517\C1,-4.916621
2447,2.1932287298,-1.8165458453\H,5.4352679028,-2.9417127541,0.3360218
697\H,0.5837183199,7.2249000886,0.917654995\\Version=ES64L-G16RevC.01\
State=1-A\HF=-1356.0684036\RMSD=9.991e-09\RMSF=3.870e-06\Dipole=0.7112
187,0.6776215,-0.0360169\Quadrupole=-1.4305895,3.4690765,-2.038487,2.0
478443,-5.0788516,3.7322376\PG=C01 [X(C19H13C11N3)]\@

Cl-Ph-Ph.cs

1\1\GINC-GADI-CPU-CLX-2071\FOpt\RM062X\6-31+G(d,p)\C19H13C11N3(1+)\FJR
502\20-Feb-2020\0\#\# M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultra
fine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\C1-Ph-Ph.cs
\1,1\C,-3.5784510919,1.4999228386,-0.9449123543\C,-3.6556952322,0.072
2677042,-0.9654540487\C,-2.5540600223,-0.6746818385,-0.6770853411\C,-1
.3267818481,-0.0263402239,-0.3493275331\C,-1.2984689598,1.4050882025,-
0.2906952738\C,-2.4377213335,2.1793895735,-0.6162880005\N,-0.103323283
3,1.9451909836,0.0727066269\N,-0.2283257568,-0.7447629808,-0.131645230
2\C,0.9002999658,-0.0921504045,0.13092412\N,0.9733153019,1.2480479044,
0.2646376631\C,0.0710756329,3.3754937233,0.2650019979\C,-0.7083733761,
4.0312108232,1.2125018563\H,-1.4465293784,3.4895143271,1.7961306238\C,
-0.4927602452,5.3933164645,1.4053753837\H,-1.0790325108,5.9259751757,2
.1464044333\C,0.4759676244,6.0638056286,0.6575369468\C,1.2452215999,5.
3781637473,-0.2837303466\H,1.9974261525,5.902690483,-0.8630736671\C,1.
0525018706,4.0142906965,-0.4848139455\H,1.6383683722,3.4562918118,-1.2
083283222\H,-4.5954165484,-0.401158151,-1.2291160703\H,-2.5692053296,-
1.7586057295,-0.704867177\H,-2.4042813927,3.261855125,-0.622228735\C,2
.1589457176,-0.8417512655,0.3136581852\C,2.1655508391,-2.2305601336,0.
13054554\H,1.2490274301,-2.7437861203,-0.1395484993\C,3.3483939235,-2.
9445612767,0.2935014887\H,3.350663125,-4.0202892375,0.1498973167\C,4.5
263239064,-2.2804210892,0.6389421606\C,4.520390731,-0.8968720729,0.821
5507352\H,5.4347184805,-0.3783355711,1.0913429532\C,3.3421418421,-0.17
4899653,0.6598891881\H,3.3394199955,0.9001408534,0.8033875147\C1,-4.99
94410033,2.3892167788,-1.3673088674\H,5.4478223961,-2.8402984268,0.765
3459431\H,0.6355824055,7.1259013297,0.8128527346\\Version=ES64L-G16Rev
C.01\State=1-A\HF=-1355.7667933\RMSD=7.894e-09\RMSF=9.285e-06\Dipole=-
0.7486394,0.6911818,-0.070082\Quadrupole=6.4342524,13.7652843,-20.1995
368,0.6184695,1.8343721,4.5147636\PG=C01 [X(C19H13C11N3)]\@

Cl-Ph-Ph.nd

1\1\GINC-GADI-CPU-CLX-2789\FOpt\UM062X\6-31+G(d,p)\C19H13C11N3(2)\FJR5
02\20-Feb-2020\0\#\# M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultraf
ine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\C1-Ph-Ph.nd\
\0,2\C,-3.6112980833,1.4704121665,-0.9378689737\C,-3.6785920307,0.0725
615884,-0.9760037777\C,-2.5401231866,-0.6583762792,-0.6871401726\C,-1.
3335810415,-0.01977730276,-0.348166427\C,-1.3123419154,1.3968914236,-0.
2839943904\C,-2.4516907099,2.1490894595,-0.6023010924\N,-0.1033325376,
1.9708558692,0.0803519733\N,-0.2082721458,-0.7647291178,-0.1150781237\
C,0.9085621547,-0.0805265912,0.1215849588\N,1.0259122297,1.2437426316,
0.2249915737\C,0.0694088443,3.3798123213,0.2671400834\C,-0.7193979628,
4.0586690437,1.1950770366\H,-1.4681984556,3.5211014079,1.7692700358\C,
-0.5211967794,5.4253817465,1.3805170097\H,-1.1287509156,5.9601721473,2

.1036297303\C,0.4610740337,6.0985161726,0.653110336\C,1.2514581424,5.4032544939,-0.2630743079\H,2.0178134923,5.9237163583,-0.828656851\C,1.0588505255,4.0380305606,-0.4615735227\H,1.6637848888,3.4801161945,-1.1693336283\H,-4.6071076535,-0.4223601385,-1.238584895\H,-2.5498839366,-1.7429342956,-0.7260939785\H,-2.4316415351,3.2321475383,-0.5942613655\C,2.1745626164,-0.8478941762,0.3056258246\C,2.1763988453,-2.2367234033,0.1320484728\H,1.2533690577,-2.7395210545,-0.1350239711\C,3.3528074486,-2.9641442461,0.2999718158\H,3.3429122066,-4.0411466277,0.1621892352\C,4.538051798,-2.3130304799,0.6423405951\C,4.5407160743,-0.9282430063,0.8163717436\H,5.4589455951,-0.414592532,1.0847088319\C,3.366863885,-0.1978126427,0.6496356619\H,3.3701923826,0.8779146265,0.788159575\C1,-5.0389874962,2.3959120585,-1.333021318\H,5.4544093378,-2.8808067996,0.7733269689\H,0.6135928269,7.1626166094,0.8038353329\Version=ES64L-G16RevC.01\State=2-A\HF=-1355.9436096\S2=0.768848\S2-1=0.\S2A=0.75021\RMSD=3.125e-09\RMSF=1.219e-05\Dipole=0.1683609,1.1612179,0.1511432\Quadrupole=-1.3546175,10.3079717,-8.9533541,2.7970502,-2.4016229,3.675331\PG=C01 [X(C19H13C11N3)]\@

3-trifluoromethyl radical

H-CF3-Ph.as

1\1\GINC-GADI-CPU-CLX-2697\FOpt\RM062X\6-31+G(d,p)\C14H9F3N3(1-)\FJR502\20-Feb-2020\0\#\M062X\6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-CF3-Ph.as\1,1\C,-3.6833346285,1.3621765169,-0.8069323853\C,-3.708351203,0.0093413197,-0.4826982131\C,-2.532333734,-0.6400127057,-0.0938173539\C,-1.3263547085,0.0595797694,0.0187023219\C,-1.3328958751,1.4543828148,-0.2370166397\C,-2.4839749362,2.0815820234,-0.7025071986\N,-0.0965023498,2.1043261045,0.0082435425\N,-0.1333238739,-0.6034350954,0.2937687797\C,0.9315191154,0.1129223769,-0.0688998066\N,1.0672938689,1.3795866919,-0.3460904891\C,0.0689924572,3.4739817887,0.1713776391\C,-0.9152356445,4.2480769808,0.8228794155\H,-1.8188119497,3.7736721305,1.1901422254\C,-0.7226961683,5.6087090307,1.0259037175\H,-1.4949451044,6.1770386881,1.5372393617\C,0.4482372428,6.243914599,0.6000515608\C,1.4301827794,5.4782149777,-0.0261215086\H,2.3534367177,5.9455107191,-0.3585842982\C,1.2546900806,4.1119673735,-0.2411530401\H,2.0295946779,3.5285025949,-0.7212620489\H,-4.6365571922,-0.5514375222,-0.5467128676\H,-2.5271427095,-1.7054349066,0.1202088924\H,-2.4644037861,3.1379069437,-0.9497762245\H,-4.5857839436,1.8702519469,-1.132708599\H,0.5920305457,7.307283088,0.7628506126\C,2.1885404166,-0.7127557875,-0.2837719055\F,2.4306958017,-1.5184016873,0.7685453754\F,2.0790742652,-1.5204687502,-1.3609028213\F,3.2941098384,0.0242979757,-0.4696780443\Version=ES64L-G16RevC.01\State=1-A\HF=-1002.4724906\RMSD=9.301e-09\RMSF=1.215e-05\Dipole=-1.1945319,2.2910043,-0.0893247\Quadrupole=2.9736383,-5.9838881,3.0102498,3.2609103,-0.5090367,0.9222153\PG=C01 [X(C14H9F3N3)]\@

H-CF3-Ph.cs

1\1\GINC-GADI-CPU-CLX-2638\FOpt\RM062X\6-31+G(d,p)\C14H9F3N3(1+)\FJR502\20-Feb-2020\0\#\M062X\6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-CF3-Ph.cs\1,1\C,-3.6657173796,1.4630286306,-0.6458062187\C,-3.6942415054,0.0369360492,-0.608172788\C,-2.5481081853,-0.6842265797,-0.4220086583\C,-1.321592839,0.0068116324,-0.2469752426\C,-1.3164911043,1.4458989816,-0.2307364592\C,-2.5079199976,2.1725480232,-0.4628382462\N,-0.1058012883,2.0341638204,-0.0078222628\N,-0.177723665,-0.6791615571,-0.1230522892\C,0.9138317712,0.0366723434,0.0084782224\N,1.0025213202,1.3655086725,0.0945537463\C,0.0519475774,3.4724074206,0.1190515419\C,-0.6823255172,4.1566073477,1.0839610127\H,-1.3750189863,3.631505143,1.7340434103\C,-0.4766195878,5.5278185924,1.2065690689\H,-1.0271119374,6.0838011608,1.9576822576\C,0.437688174,6.1788734463,0.3769814705\C,1.1656305136,5.4642175956,-0.5755020518\H,1.8779252236,5.9729775919,-1.2159791757\C,0.9845587387,4.0909331953,-0.7074343712\H,1.5420867539,3.5099206751,-1.4349412531\H,-4.6407989114,-0.4730316585,-0.7511946992\H,-2.5284393166,-1.768437203,-0.4176150288\H,-2.5003638458,3.2538002827,-0.5111088204\H,-4.5886786275,2.001183561,-0.8337988129\H,0.5879110442,7.2489093934,0.477

4544601\C,2.2586758883,-0.6702220384,0.1277921549\F,2.1261147475,-1.98
2017654,-0.0367760916\F,3.1119544048,-0.2093709898,-0.793652294\F,2.80
1856537,-0.4467758786,1.3301274178\\Version=ES64L-G16RevC.01\State=1-A
\HF=-1002.1563886\RMSD=8.319e-09\RMSF=1.077e-05\Dipole=-3.8873138,1.79
4954,-0.4808873\Quadrupole=7.2020381,6.6639842,-13.8660223,8.5617488,-
0.420626,2.8160369\PG=C01 [X(C14H9F3N3)]\@

H-CF3-Ph.nd

1\1\GINC-GADI-CPU-CLX-2085\FOpt\UM062X\6-31+G(d,p)\C14H9F3N3(2)\FJR502
\21-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafin
e) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-CF3-Ph.nd.nd
\0,2\C,0.8940470042,3.6402369874,-0.2392566635\C,-0.4467441995,4.0361
764923,-0.1129466983\C,-1.4419381746,3.0831431574,0.0183124044\C,-1.11
82416841,1.7162249035,0.0397526009\C,0.2450195245,1.3303804161,-0.0523
639476\C,1.2459137664,2.2984651522,-0.2137884764\N,0.5116931192,-0.036
7054707,-0.0001853824\N,-2.12000541,0.7768120209,0.1211730304\C,-1.699
1004046,-0.4748357273,0.0639276694\N,-0.4749158263,-0.9577808712,0.003
3848562\C,1.8369168535,-0.5812042191,-0.0047515255\C,2.7418401144,-0.2
108546071,0.989335304\H,2.4451371194,0.4943233373,1.7599949902\C,4.018
5473396,-0.7685311453,0.98194448\H,4.7285453838,-0.4886444271,1.753598
4572\C,4.3768998721,-1.6916285602,-0.0013730957\C,3.4556350066,-2.0622
447249,-0.9816880811\H,3.7307152448,-2.7825249313,-1.745530071\C,2.178
0156925,-1.5070958287,-0.9889524224\H,1.4475726377,-1.7837276886,-1.74
26658766\H,-0.7035288772,5.0902575464,-0.1305428805\H,-2.4891306156,3.
3578743786,0.0965806365\H,2.2827552877,2.0034298272,-0.3226344873\H,1.
670536308,4.3879737571,-0.3634016098\H,5.371952959,-2.1253780152,-0.00
05280239\C,-2.8032120658,-1.5192361508,0.0903777419\F,-3.6536241708,-1
.3439342895,-0.9350025107\F,-2.338493104,-2.7693760268,0.01814179\F,-3
.5274087008,-1.4206852925,1.2179977916\\Version=ES64L-G16RevC.01\State
=2-A\HF=-1002.341962\S2=0.76692\S2-1=0.\S2A=0.750169\RMSD=9.279e-09\R
MSF=3.531e-06\Dipole=3.087825,1.501424,-0.1681191\Quadrupole=-1.2119544
,4.6095373,-3.3975829,-5.1317886,1.5111504,2.8947241\PG=C01 [X(C14H9F3
N3)]\@

1-(4-trifluoromethylphenyl) radical

H-Ph-PhCF3.as

1\1\GINC-GADI-CPU-CLX-2647\FOpt\RM062X\6-31+G(d,p)\C20H13F3N3(1-)\FJR5
02\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafin
e) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-Ph-PhCF3.a
s\ -1,1\C,-3.6781287961,1.1471429331,-0.8499919851\C,-3.662303519,-0.1
169455985,-0.2580678584\C,-2.4695342522,-0.6568865656,0.2224712746\C,-
1.2683878256,0.0683236308,0.1540442682\C,-1.3227935259,1.3828518046,-0
.3665173685\C,-2.4957540121,1.8916279823,-0.9184459958\N,-0.0950116802
,2.0824327287,-0.3029579867\N,-0.0621355818,-0.5044998639,0.5131813436
\C,1.0078948529,0.1182975023,-0.0054954937\N,1.0728616947,1.3192106788
, -0.5497086445\C,0.0717294132,3.4072179827,-0.0191891775\C,-0.98827752
86,4.2213996078,0.4581893577\H,-1.9700354577,3.7972971389,0.6254745277
\C,-0.7784083156,5.5576387379,0.7547824465\H,-1.6066192613,6.149732218
9,1.1318977814\C,0.4820014975,6.1390428551,0.588920593\C,1.5399895892,
5.3466581431,0.1307102919\H,2.5280749244,5.7821658095,0.0026629816\C,1
.3515348644,4.0078274159,-0.1630913043\H,2.1800770823,3.4040425268,-0.
5063959631\H,-4.5798451962,-0.6946145555,-0.1867174735\H,-2.4405813704
, -1.656794906,0.6477217547\H,-2.4951519736,2.8771415115,-1.3744472055\
C,2.295116075,-0.6545224612,-0.0323168213\C,2.2960000764,-2.0357987369
,0.1920429138\H,1.352057251,-2.5363250917,0.3791760397\C,3.4897176645,
-2.7569341114,0.1737800627\H,3.4736350484,-3.8289315586,0.348779359\C,
4.699312624,-2.1070741896,-0.0716870456\C,4.7072475391,-0.728743651,-0
.2941897869\H,5.6449345236,-0.2129140935,-0.4802594587\C,3.5151852419,
-0.0080760981,-0.2707481609\H,3.52076944,1.0649896148,-0.4321819483\H,
5.6291159195,-2.6684643489,-0.0867932634\H,-4.599204169,1.5591231814,-
1.2502714908\C,0.7187591433,7.5788881679,0.8692655884\F,0.9884224724,8
.3024818381,-0.2498516103\F,-0.3338623871,8.1831275891,1.4558924417\F,
1.7830679147,7.7896442304,1.6825330169\\Version=ES64L-G16RevC.01\State
=1-A\HF=-1233.4579316\RMSD=3.999e-09\RMSF=2.934e-06\Dipole=0.2589707,0

.7138795,-0.1489281\Quadrupole=19.1874254,-24.351113,5.1636876,-5.720104,-0.6784818,-3.9308479\PG=C01 [X(C20H13F3N3)]\ \@

H-Ph-PhCF3.cs

1\1\GINC-GADI-CPU-CLX-2647\FOpt\RM062X\6-31+G(d,p)\C20H13F3N3(1+)\FJR502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-Ph-PhCF3.cs\1,1\C,-3.6153157967,1.4109856227,-0.6603945529\C,-3.6328679546,-0.018415199,-0.6413395803\C,-2.4863989652,-0.7352416784,-0.4542449856\C,-1.2568413962,-0.0422901735,-0.2653239738\C,-1.2672842461,1.3928459365,-0.2396042728\C,-2.462984299,2.1213916188,-0.4641237127\N,-0.0607685148,1.9724079087,-0.0093694288\N,-0.1162542331,-0.7188078519,-0.1348021834\C,1.0094755402,-0.0274674329,0.01091184\N,1.0537476949,1.3183696254,0.101535515\C,0.085819444,3.413210235,0.1264680414\C,-0.5893242288,4.0652195337,1.1493227085\H,-1.232100926,3.5168266209,1.8307891426\C,-0.4041078218,5.4385390999,1.287810138\H,-0.9108802358,5.9733439046,2.0828723472\C,0.4392633132,6.1070889364,0.405055202\C,1.1115522527,5.4321218641,-0.6154877952\H,1.7649343302,5.9712077689,-1.2945915138\C,0.9412646663,4.0613117886,-0.7577313564\H,1.4529235148,3.5050739357,-1.5361108808\H,-4.5758390958,-0.5320170544,-0.7949616152\H,-2.4653983478,-1.8195763262,-0.457688728\H,-2.458389537,3.2037573461,-0.4925287857\C,2.3022337031,-0.7358069886,0.1022323832\C,2.3310847034,-2.1318712807,-0.0081292071\H,1.4069735143,-2.6805240805,-0.1539807855\C,3.5447779601,-2.8077077969,0.0682855877\H,3.5634680264,-3.889338152,-0.0184955808\C,4.7321579551,-2.0981353489,0.254277384\C,4.7042087595,-0.7073007082,0.3649424752\H,5.6258885082,-0.1531737531,0.5106583572\C,3.4947461571,-0.0236178965,0.2896122165\H,3.476415801,1.0572084772,0.3777180021\H,5.6778305694,-2.6283551507,0.3128322198\H,-4.5418732602,1.9453677918,-0.8409849464\C,0.6554810179,7.5914411598,0.53177691\F,0.2955200846,8.2431359385,-0.5907728847\F,-0.043256001,8.1308082616,1.5411982669\F,1.9515873438,7.8887634975,0.7445680325\Version=ES64L-G16RevC.01\State=1-A\HF=-1233.153324\RMSD=6.184e-09\RMSF=3.546e-05\Dipole=-2.8949999,-2.5912155,-0.6452901\Quadrupole=22.2485182,-5.305048,-16.9434702,1.1271094,1.2153106,1.9294377\PG=C01 [X(C20H13F3N3)]\ \@

H-Ph-PhCF3.nd

1\1\GINC-GADI-CPU-CLX-1741\FOpt\UM062X\6-31+G(d,p)\C20H13F3N3(2)\FJR502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-Ph-PhCF3.nd\0,2\C,-3.6620072522,1.3660662437,-0.653966493\C,-3.6682238884,-0.0370738349,-0.5986561004\C,-2.4877940782,-0.7278372762,-0.388926646\C,-0.2742823439,-0.0363825369,-0.2137967854\C,-1.292835761,1.381087292,-0.2253129577\C,-2.4851366325,2.0776179261,-0.4736793724\N,-0.0665801887,2.0035616179,-0.01307733\N,-0.105586618,-0.738328654,-0.0664877193\C,1.0083466999,-0.0151527399,0.002695\N,1.0955229669,1.3155616105,0.0291692536\C,0.0846204569,3.4149223178,0.1249515528\C,-0.6866334129,4.1117779097,1.053900127\H,-1.4088144155,3.5858866783,1.6698815227\C,-0.506653277,5.4845781019,1.1985818363\H,-1.0981295839,6.0331506051,1.9232539005\C,0.4472313062,6.1373093367,0.4223534718\C,1.2283932823,5.4345555604,-0.497533434\H,1.9700293645,5.95423214,-1.0970175829\C,1.0492888304,4.0662068238,-0.6472826102\H,1.6456903611,3.4988409783,-1.3534661847\H,-4.5980386236,-0.5797336687,-0.7351941\H,-2.4598405296,-1.8129120969,-0.366756358\H,-2.4896186439,3.1597514239,-0.5312897012\C,2.3117379206,-0.7385468827,0.07460199\C,2.3364829661,-2.1356940271,-0.004883486\H,1.4039734029,-2.6777097153,-0.1176092085\C,3.5473834283,-2.8219644933,0.0599997048\H,3.5544024556,-3.9059524172,-0.0030586618\C,4.744923921,-2.121154218,0.204006701\C,4.7250032198,-0.7279484313,0.2835085455\H,5.6528677846,-0.1755625968,0.3973226865\C,3.5165764479,-0.0386972614,0.2197751353\H,3.5033269764,1.043859966,0.2851907266\H,5.6882099548,-2.6568710959,0.2544674305\H,-4.5834723508,1.9065398388,-0.8445151269\C,0.6570096566,7.6176628113,0.5482216905\F,0.3409320293,8.2703728938,-0.5911581365\F,-0.0809850708,8.1678319504,1.526072538\F,1.9441492387,7.9269279202,0.8079202123\Version=ES64L-G16RevC.01\State=2-A\HF=-1233.3293838\S2=0.768574\S2-1=0.\S2A=0.750206\RMSD=8.403e-09\RMSF=3.446e-06\Dip

ole=-1.0510796,-0.0486363,-0.2017476\Quadrupole=17.3945209,-13.9148161
,-3.4797049,-2.5643438,-1.7216194,-0.0794064\PG=C01 [X(C20H13F3N3)]\@

1-(4-chlorophenyl) radical

H-Ph-PhCl.as

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1\1\GINC-GADI-CPU-CLX-1741\FOpt\RM062X\6-31+G(d,p)\C19H13Cl1N3(1-)\FJR
502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultra
fine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-Ph-PhCl.a
s\1,1\C,-3.6037641234,1.3220674559,-1.1819405107\C,-3.6970299743,-0.
0082510923,-0.7772159591\C,-2.5931998242,-0.6506217803,-0.2113765162\C
,-1.3854430555,0.0321578437,-0.0032065856\C,-1.3359202616,1.4069359834
,-0.3431853968\C,-2.4091251307,2.0256035113,-0.9791905204\N,-0.1187933
814,2.0380669683,-0.0047594898\N,-0.2571790294,-0.6268344315,0.4546341
198\C,0.8914186444,0.0134031736,0.1773792769\N,1.0591712246,1.26925863
27,-0.1845259113\C,0.0532782204,3.3761256259,0.2658043671\C,-1.0137390
705,4.1866975545,0.7210317092\H,-1.9995445546,3.7602088192,0.863705735
7\C,-0.8155203224,5.5254947369,1.0266628741\H,-1.6470583394,6.12477784
71,1.3845936875\C,0.45086568,6.0906207588,0.8893546505\C,1.5214943688,
5.3151920848,0.4621329513\H,2.5097156413,5.754036839,0.3626686809\C,1.
3303317805,3.9711798019,0.1558300063\H,2.1673782801,3.3694977809,-0.17
22594043\H,-4.6247207009,-0.5565819035,-0.9165224422\H,-2.6432479606,-
1.6989594387,0.0715153575\H,-2.3310721046,3.0630484115,-1.2892646474\C
,2.1500533257,-0.8039741163,0.2270069402\C,2.0815708166,-2.2011553109,
0.2622424495\H,1.1062002137,-2.6755809569,0.2476252326\C,3.2455000094,
-2.9682278536,0.311715527\H,3.1754639994,-4.0519999029,0.3371451815\C,
4.494918682,-2.3483053641,0.3250199986\C,4.5718974597,-0.9544731968,0.
2929330951\H,5.5402547236,-0.4624674269,0.3094618353\C,3.4088628186,-0
.1887449405,0.2482172789\H,3.4668522481,0.8947178603,0.2361356321\H,-4
.4494847584,1.8205776976,-1.6455606188\H,5.4016942568,-2.9452068282,0.
3628579897\Cl,0.6932101983,7.7900151561,1.2670434253\Version=ES64L-G1
6RevC.01\State=1-A\HF=-1356.0680547\RMSD=8.447e-09\RMSF=1.009e-05\Dipo
le=0.5011944,0.7269657,-0.1305354\Quadrupole=13.9723311,-16.0466252,2.
0742941,-4.9289209,-0.0409368,-2.7992936\PG=C01 [X(C19H13Cl1N3)]\@
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H-Ph-PhCl.cs

```
1\1\GINC-GADI-CPU-CLX-1749\FOpt\RM062X\6-31+G(d,p)\C19H13Cl1N3(1+)\FJR
502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultra
fine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-Ph-PhCl.c
s\1,1\C,-3.6073426221,1.5141782055,-0.9601516258\C,-3.6640774576,0.08
70586903,-1.0161994608\C,-2.5604508955,-0.6727221936,-0.7551961075\C,-
1.3384483409,-0.0281010148,-0.4111188792\C,-1.3126780131,1.4036608384,
-0.3170058684\C,-2.4614208201,2.1786197138,-0.6181301764\N,-0.11755452
96,1.935236058,0.0524499513\N,-0.2363908594,-0.7472180154,-0.198533008
\C,0.8859361098,-0.0996060665,0.0952783337\N,0.9600671454,1.2396867978
,0.245208091\C,0.057633423,3.3636397773,0.2553289122\C,-0.6625940381,3
.9995054964,1.2597045254\H,-1.362660128,3.4469407175,1.8786311594\C,-0
.4528910115,5.3586927797,1.4666269154\H,-0.9921971517,5.8826636327,2.2
479289649\C,0.4643258741,6.032568556,0.6631763962\C,1.1856260556,5.384
7326375,-0.3377110017\H,1.8951694739,5.9309625885,-0.9493296551\C,0.98
4842054,4.0239150948,-0.5413543217\H,1.5320171748,3.4878351284,-1.3102
485579\H,-4.6003380325,-0.3894420627,-1.2867231358\H,-2.5667494099,-1.
7557206812,-0.8108383067\H,-2.42674238,3.26074026,-0.5922485198\C,2.13
92224482,-0.8537351035,0.3015839913\C,2.1386281832,-2.2455050371,0.144
0046652\H,1.2214153731,-2.7568106187,-0.1273186749\C,3.3137784749,-2.9
648781819,0.3364527507\H,3.3100858137,-4.0430848969,0.2134293237\C,4.4
917208354,-2.3029038719,0.6859044306\C,4.4931594251,-0.916277783,0.842
5641804\H,5.4077068995,-0.3994980105,1.1151885375\C,3.32242079,-0.1890
831855,0.6516169759\H,3.3255581205,0.8883359696,0.7758860642\H,-4.4975
158392,2.0849184364,-1.2025660038\H,5.4071675902,-2.8669669552,0.83624
2412\Cl,0.7188602646,7.7359622998,0.9211767227\Version=ES64L-G16RevC.
01\State=1-A\HF=-1355.7694315\RMSD=8.620e-09\RMSF=6.600e-06\Dipole=-2.
6946671,-0.8433375,-0.8380007\Quadrupole=19.0223429,-1.6140803,-17.408
2626,-1.9090879,5.0891342,1.8578994\PG=C01 [X(C19H13Cl1N3)]\@
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H-Ph-PhCl.nd

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1\1\GINC-GADI-CPU-CLX-0088\FOpt\UM062X\6-31+G(d,p)\C19H13Cl1N3(2)\FJR502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-Ph-PhCl.nd\0,2\C,-3.6511300934,1.4777598134,-0.9470677474\C,-3.7005838264,0.0748862565,-0.9710823083\C,-2.5660890725,-0.6640108679,-0.6830056577\C,-1.3580894239,-0.0227114108,-0.3518631275\C,-1.3348955155,1.3936647053,-0.2940792919\C,-2.4783594259,2.1404443523,-0.6152508679\N,-0.1194505081,1.9660502576,0.0643421738\N,-0.23134115,-0.7690490115,-0.1172067287\C,0.8874998134,-0.0867231942,0.1090598731\N,1.0106322788,1.2383131241,0.2036146861\C,0.0572608489,3.3705540139,0.2538935316\C,-0.7389791708,4.0570902035,1.1699531855\H,-1.5014174698,3.5301285621,1.735062442\C,-0.541011927,5.4203303002,1.3674026842\H,-1.1501975816,5.9659772807,2.0797643108\C,0.4608460279,6.068882137,0.6510441588\C,1.2700596823,5.388114508,-0.2543280977\H,2.0472024223,5.9120365981,-0.8002796077\C,1.0640321036,4.0264122225,-0.4529572137\H,1.6810117056,3.4715159323,-1.1520758781\H,-4.6265071554,-0.4296141802,-1.2277558453\H,-2.5708524012,-1.7492327782,-0.7146926622\H,-2.447341596,3.2236656846,-0.6116681833\C,2.1523151291,-0.8570927982,0.2931478757\C,2.1569139321,-2.2422470276,0.0924459978\H,1.2374969067,-2.7392901513,-0.1971125273\C,3.33085425,-2.9732237298,0.2619986458\H,3.322820423,-4.0472307889,0.1024052194\C,4.5113032888,-2.3293567767,0.6335554552\C,4.511379866,-0.9483354732,0.8348617789\H,5.4257351346,-0.4405899635,1.1267811073\C,3.3398869507,-0.2144231168,0.6659500006\H,3.3410665286,0.8581535237,0.8270794602\H,-4.5349311555,2.0568389278,-1.1944499409\H,5.4255849446,-2.9001090257,0.7664141832\C,0.7125652361,7.7807218908,0.8998089155\Version=ES64L-G16RevC.01\State=2-A\HF=-1355.9439545\S2=0.768368\S2-1=0.\S2A=0.750199\RMSD=4.651e-09\RMSF=3.509e-06\Dipole=-0.8841807,0.6234217,-0.2385884\Quadrupole=13.2047042,-7.217496,-5.9872082,-3.4029669,0.3259225,0.1583128\PG=C01 [X(C19H13Cl1N3)]\@
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1-(4-methylphenyl) radical

H-Ph-PhMe.as

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1\1\GINC-GADI-CPU-CLX-0090\FOpt\RM062X\6-31+G(d,p)\C20H16N3(1-)\FJR502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-Ph-PhMe.as\ -1,1\C,-3.5889053583,1.2540799404,-0.8630794841\C,-3.6142035453,-0.0839026355,-0.4796171638\C,-2.45063807,-0.7009326405,-0.0088950349\C,-1.253113133,0.0149780001,0.1252187618\C,-1.266246248,1.3980709693,-0.1920934319\C,-2.4021926821,1.9914926323,-0.7353162387\N,-0.0490466157,2.0583225751,0.0907563981\N,-0.0763079393,-0.615350248,0.4954500483\C,1.0298214638,0.0626412701,0.1378844919\N,1.1320848851,1.3275974547,-0.2079776582\C,0.1000807408,3.4371684,0.1765003037\C,-0.9092363709,4.2414470664,0.7510752401\H,-1.8211414348,3.7813680647,1.117104597\C,-0.735399418,5.6115494635,0.8812790473\H,-1.5312539454,6.1990536094,1.3355353109\C,0.4407009574,6.2544320495,0.4633517435\C,1.4416913641,5.4505253383,-0.0814319776\H,2.3735820449,5.9085239064,-0.4073077936\C,1.2887361263,4.0698717982,-0.2275601544\H,2.0871462391,3.4733955508,-0.6499256288\C,2.3100025469,-0.7178883202,0.0685515277\C,2.2828740326,-2.1161549323,0.0196232139\H,1.321691426,-2.619137538,0.0277977832\C,3.4688745588,-2.847690734,-0.0433411576\H,3.4308549436,-3.9326714077,-0.0834825796\C,4.6993603048,-2.1908648885,-0.0584224723\H,5.6231939383,-2.7601486327,-0.1071511553\C,4.7352766196,-0.7958875955,-0.0058573164\H,5.6888938236,-0.2755541062,-0.0100869891\C,3.5503585656,-0.066131954,0.0606041521\H,3.5751648849,1.0176653306,0.1124554378\H,-4.5333626774,-0.6580286246,-0.5592851488\H,-2.4472762256,-1.7548252772,0.2579517452\H,-2.3828310542,3.0373080338,-1.0244921066\H,-4.4809135257,1.7364410131,-1.2513391699\C,0.6023626366,7.7469188987,0.6066251078\H,-0.109684712,8.2882031608,-0.0266119151\H,0.4286665878,8.0697551845,1.6388975846\H,1.6099542651,8.0610798244,0.3203720817\Version=ES64L-G16RevC.01\State=1-A\HF=-935.7946615\RMSD=3.162e-09\RMSF=8.838e-06\Dipole=0.6959327,1.8253006,-0.1718245\Quadrupole=4.491885,-0.5056483,-3.9862368,-3.2005048,-0.8095969,2.182967\PG=C01 [X(C20H16N3)]\@
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H-Ph-PhMe.cs

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1\1\GINC-GADI-CPU-CLX-1626\FOpt\RM062X\6-31+G(d,p)\C20H16N3(1+)\FJR502
\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafin
e) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-Ph-PhMe.cs\
1,1\C,-3.6114413428,1.4212690654,-0.6720194707\C,-3.6342206064,-0.0063
071048,-0.6173408845\C,-2.4888620937,-0.7220923386,-0.4165174317\C,-1.
2568562287,-0.0293571647,-0.2475917802\C,-1.2619086455,1.4046186031,-0
.2509213271\C,-2.4557244416,2.1313712322,-0.4933729503\N,-0.0533946092
,1.9884037824,-0.0271058191\N,-0.1169684881,-0.7094541533,-0.112567016
\C,1.0095379934,-0.0178947941,0.0081945364\N,1.0581304805,1.3294125554
,0.0822241199\C,0.0922480931,3.4254035558,0.1072247187\C,-0.6180538777
,4.0926494321,1.098875868\H,-1.2893533276,3.5528654773,1.7601103554\C,
-0.4205433624,5.4628194732,1.2388239929\H,-0.9549259917,5.9979356008,2
.0182776696\C,0.4629929346,6.1575769435,0.4036571053\C,1.1645867119,5.
4442341804,-0.5783727013\H,1.8580972632,5.9687831523,-1.2293812832\C,0
.9935876959,4.0737240835,-0.7308031886\H,1.5378566069,3.514696116,-1.4
856257029\C,2.3031283859,-0.7264414248,0.0996466008\C,2.3332336844,-2.
1222908129,-0.0136278444\H,1.4098513078,-2.6707528872,-0.1652169892\C,
3.5467641524,-2.7981076085,0.0671905385\H,3.5666609022,-3.8795711808,-
0.0218846892\C,4.7330323621,-2.0887714634,0.261016703\H,5.6784286481,-
2.6189729299,0.3238677815\C,4.7039238539,-0.6982281242,0.374064582\H,5
.6243915841,-0.1438990291,0.5262726305\C,3.4945796159,-0.0146304889,0.
2937862356\H,3.4749368856,1.0659629673,0.384462142\H,-4.5789396773,-0.
5207674433,-0.7573456629\H,-2.4699883822,-1.8062840751,-0.3963144886\H
,-2.4460797285,3.2125955926,-0.5510780349\H,-4.5353310877,1.9546268336
,-0.8685902412\C,0.6466032984,7.6439850248,0.5425730641\H,0.0445669017
,8.1714569707,-0.2055024846\H,0.3344084909,7.9898660505,1.5304752425\H
,1.6906640382,7.9262863305,0.3841961039\Version=ES64L-G16RevC.01\Stat
e=1-A\HF=-935.5035088\RMSD=5.304e-09\RMSF=7.620e-06\Dipole=-2.5178221,
0.9543551,-0.382306\Quadrupole=13.4666953,11.7897624,-25.2564577,-1.49
11841,1.5236178,2.7042669\PG=C01 [X(C20H16N3)]\@
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H-Ph-PhMe.nd

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1\1\GINC-GADI-CPU-CLX-2429\FOpt\UM062X\6-31+G(d,p)\C20H16N3(2)\FJR502\
20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine
) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-Ph-PhMe.nd\0
,2\C,-3.6525083145,1.3874539909,-0.6536781192\C,-3.6608999383,-0.01592
33982,-0.6222010687\C,-2.4812899962,-0.712108223,-0.4204219785\C,-1.26
72168345,-0.0263843208,-0.2320204868\C,-1.2818659242,1.3916605173,-0.2
269612047\C,-2.4739095412,2.093863758,-0.4614726122\N,-0.0580476473,2.
0117282869,-0.0063928738\N,-0.0997515581,-0.7322319867,-0.0849017056\C
,1.0128370452,-0.0093860008,0.0087088965\N,1.1013423334,1.320803215,0.
05012875\C,0.0899522832,3.4285609433,0.1223880358\C,-0.6283924337,4.12
27399218,1.0923805809\H,-1.3138130279,3.5922122416,1.746801915\C,-0.44
69157145,5.4989401208,1.2202682164\H,-1.004569542,6.039455045,1.980259
5117\C,0.4506143753,6.1909624447,0.4012933428\C,1.1700679804,5.4655573
191,-0.5583927849\H,1.8754581023,5.9846668002,-1.2025299698\C,0.996691
8556,4.0937478927,-0.7035305625\H,1.5564708132,3.5329769095,-1.4455813
368\C,2.3152051601,-0.7346269535,0.0901626115\C,2.3417643503,-2.130527
1802,-0.0087612447\H,1.410956329,-2.6705800893,-0.1428291122\C,3.55174
27213,-2.8179044305,0.0637222906\H,3.5600027295,-3.9009080795,-0.01488
08653\C,4.747068095,-2.1194724443,0.2349718241\H,5.6895621237,-2.65601
23105,0.29129685\C,4.725522856,-0.727496897,0.3340581353\H,5.651409808
7,-0.1765034755,0.4690194708\C,3.5179731327,-0.0373494345,0.2624317059
\H,3.5030722365,1.0442030816,0.342149825\H,-4.5911297426,-0.5553655295
,-0.7687567306\H,-2.4557823178,-1.7974958961,-0.4131769813\H,-2.474630
3294,3.1769261067,-0.49768681\H,-4.5734417013,1.9324146677,-0.83412235
78\C,0.6500396167,7.6775853923,0.5399043246\H,0.365110629,8.1955534289
,-0.3817132514\H,0.0499530773,8.0818987738,1.3584357937\H,1.7009669092
,7.9130857919,0.7353899761\Version=ES64L-G16RevC.01\State=2-A\HF=-935
.6749894\S2=0.768104\S2-1=0.\S2A=0.750194\RMSD=7.367e-09\RMSF=2.631e-0
6\Dipole=-0.7264974,1.8963671,-0.0646489\Quadrupole=5.709957,7.1485389
,-12.8584959,-1.8505419,-0.9994542,1.6678443\PG=C01 [X(C20H16N3)]\@
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1-(4-nitrophenyl) radical

H-Ph-PhNO2.as

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1\1\GINC-GADI-CPU-CLX-0090\FOpt\RM062X\6-31+G(d,p)\C19H13N4O2(1-)\FJR5
02\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultraf
ine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-Ph-PhNO2.a
s\1,1\C,-3.6489631533,1.1933173997,-0.8614224847\C,-3.6440230711,-0.
0766887306,-0.2772939084\C,-2.4619216988,-0.6251693739,0.2127599772\C,
-1.2559974231,0.0961814515,0.1609645661\C,-1.3036221722,1.4150653718,-
0.343896158\C,-2.4671450329,1.935453971,-0.906754967\N,-0.0706282,2.11
19651668,-0.2630938221\N,-0.0564004676,-0.4894681384,0.5140332576\C,1.
0166192994,0.1359698358,0.012164369\N,1.0897835545,1.3485956746,-0.511
6871076\C,0.0916591731,3.4250515857,0.0167854893\C,-0.9823619047,4.244
0475456,0.481355272\H,-1.9610676177,3.8147059025,0.6503499315\C,-0.781
1340695,5.5738190915,0.766357369\H,-1.5986958202,6.1799507549,1.139458
0296\C,0.4884218086,6.1488085319,0.5936200838\C,1.5657695582,5.3621658
172,0.160642446\H,2.5451681308,5.8118995625,0.0423049628\C,1.380147049
5,4.0265280735,-0.1144164592\H,2.2105721107,3.4178961302,-0.4433094562
\C,2.300325982,-0.6391864121,-0.0235016561\C,2.2874582069,-2.029334789
9,0.1353152055\H,1.3363279573,-2.5302581734,0.2803964094\C,3.476639905
8,-2.7566884601,0.1037936418\H,3.4515244389,-3.8357029431,0.2262610501
\C,4.694186376,-2.1030473325,-0.0875353519\C,4.7151919444,-0.715906312
6,-0.2436599138\H,5.6594944196,-0.1985239026,-0.3865962121\C,3.5271357
702,0.0111132869,-0.2092994928\H,3.5412019495,1.0905799771,-0.31988080
72\H,-4.5641707748,-0.6519642985,-0.2248005769\H,-2.4399302948,-1.6300
059426,0.6259460433\H,-2.4561279659,2.922723984,-1.3584267685\H,5.6207
418393,-2.669413084,-0.1123258023\H,-4.5629712316,1.6083580057,-1.2739
995253\N,0.6847139337,7.531288154,0.8753112222\O,-0.2809343105,8.20813
08218,1.2390738765\O,1.8137318001,8.0122617983,0.7474672673\Version=E
S64L-G16RevC.01\State=1-A\HF=-1100.947075\RMSD=8.910e-09\RMSF=2.314e-0
6\Dipole=-0.1211686,-2.1683531,-0.6859326\Quadrupole=27.8735566,-41.94
15615,14.0680049,-6.1122099,0.3887462,-8.9900028\PG=C01 [X(C19H13N4O2)
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H-Ph-PhNO2.cs

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1\1\GINC-GADI-CPU-CLX-0108\FOpt\RM062X\6-31+G(d,p)\C19H13N4O2(1+)\FJR5
02\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultraf
ine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-Ph-PhNO2.c
s\1,1\C,-3.6028361531,1.4375946689,-0.6928289967\C,-3.6168081747,0.00
77225046,-0.7028107875\C,-2.4703078982,-0.7099719637,-0.5214333404\C,-
1.2439542305,-0.0178494263,-0.3081812533\C,-1.257670268,1.4173717563,-
0.260781651\C,-2.4537653531,2.1475197741,-0.4771333413\N,-0.0533284023
,1.9941561058,-0.0157279767\N,-0.1046821525,-0.6936420097,-0.171453573
3\C,1.0185033507,-0.0041028579,0.0049833816\N,1.0611193018,1.340861777
6,0.105045487\C,0.093992868,3.4357032903,0.1186732025\C,-0.542032008,4
.0823438487,1.1722885761\H,-1.1537239237,3.5301513011,1.8786030423\C,-
0.3598778914,5.4540140707,1.3069043549\H,-0.8281860802,6.0013672926,2.
1157343496\C,0.447739888,6.1049887666,0.3827853301\C,1.0867204654,5.45
79521552,-0.6674714664\H,1.7062220189,6.0107410519,-1.3630982689\C,0.9
087719959,4.0858483592,-0.8001142206\H,1.3884356198,3.5329455814,-1.60
06592161\C,2.3074061638,-0.715710596,0.1186471887\C,2.3324444289,-2.11
17531895,0.0058773957\H,1.4090120563,-2.6556655225,-0.1601949626\C,3.5
412286257,-2.7929233026,0.1067561908\H,3.5576112235,-3.8744739335,0.01
86041524\C,4.7271541214,-2.0887221071,0.3195535906\C,4.702959473,-0.69
79045496,0.4320722324\H,5.6236516451,-0.1480726414,0.5982460854\C,3.49
84407462,-0.0087259444,0.3324319586\H,3.482905321,1.0720645056,0.42150
21278\H,-4.5578751348,-0.504517848,-0.871948307\H,-2.4470829559,-1.793
9462909,-0.5436071071\H,-2.4528136409,3.2305351912,-0.4845399634\H,5.6
691167969,-2.6229293765,0.3977161849\H,-4.5304181999,1.9725112037,-0.8
670157627\N,0.6412657956,7.5603500857,0.5277953546\O,0.0320549194,8.12
72540855,1.4170799394\O,1.399325642,8.1114341829,-0.2498399303\Versio
n=ES64L-G16RevC.01\State=1-A\HF=-1100.6317249\RMSD=5.523e-09\RMSF=4.91
9e-06\Dipole=-2.9743078,-2.8883178,-0.7459841\Quadrupole=28.2310849,-1
7.3065661,-10.9245188,-1.7306868,3.1788949,-0.5288911\PG=C01 [X(C19H13
N4O2)]\@
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H-Ph-PhNO2.nd

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1\1\GINC-GADI-CPU-CLX-0108\FOpt\UM062X\6-31+G(d,p)\C19H13N4O2(2)\FJR50
2\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafi
ne) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-Ph-PhNO2.nd
\0,2\C,-3.6561874508,1.3775368948,-0.6764918514\C,-3.66363739,-0.0241
333036,-0.5843327145\C,-2.4852491545,-0.709128858,-0.3513159412\C,-1.2
72277877,-0.0128123863,-0.1867679612\C,-1.2912255817,1.4040303027,-0.2
271217298\C,-2.4811924694,2.0932945775,-0.5054102546\N,-0.0639749662,2
.0305131193,-0.0194264399\N,-0.1049913495,-0.7119754702,-0.025917495\C
,1.010577346,0.0107865223,0.0146613626\N,1.0982580828,1.3416123023,0.0
153449103\C,0.0908845245,3.4369137516,0.1128099676\C,-0.735065234,4.15
67928221,0.9818996339\H,-1.4994281877,3.6491903089,1.5601672251\C,-0.5
513511197,5.5252322607,1.1234650158\H,-1.1717545197,6.1022903705,1.798
4729116\C,0.4635012126,6.1392860477,0.3966588173\C,1.3064612898,5.4352
227653,-0.4573655346\H,2.0870179564,5.9484054051,-1.0059290177\C,1.117
2228872,4.0678067141,-0.5966745996\H,1.7535198274,3.4851930312,-1.2529
910571\C,2.3137492239,-0.7121676986,0.0820064229\C,2.3406577433,-2.105
7331424,-0.0452240365\H,1.4105822208,-2.6437857142,-0.191943704\C,3.55
09955309,-2.7931287275,0.0141253025\H,3.5605335264,-3.8741500008,-0.08
72844492\C,4.7452734188,-2.0969662872,0.2008931417\C,4.7230157473,-0.7
07342114,0.3285867319\H,5.6483458477,-0.1590503998,0.4770328755\C,3.51
51283078,-0.0167248884,0.2695956544\H,3.4993413336,1.0628844512,0.3735
382906\H,-4.5927146519,-0.5697058028,-0.7135152341\H,-2.4559512537,-1.
7933316818,-0.3047359596\H,-2.4866971254,3.1727741313,-0.5971565683\H,
5.6882228643,-2.6335715555,0.2475871387\H,-4.5757030498,1.9125854639,-
0.8899309811\N,0.6578605112,7.5846273538,0.5436460181\O,-0.111723871,8
.196414384,1.2674872927\O,1.5786958493,8.1048350505,-0.065983184\Version=ES64L-G16RevC.01\State=2-A\HF=-1100.8103046\S2=0.769072\S2-1=0.\S2
A=0.750227\RMSD=8.954e-09\RMSF=5.370e-06\Dipole=-1.1941052,-1.206052,-
0.3872259\Quadrupole=23.7597768,-25.3570015,1.5972247,-4.2898697,0.111
6966,-2.0969879\PG=C01 [X(C19H13N4O2)]\@
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1-(4-methoxyphenyl) radical

H-Ph-PhOMe.as

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1\1\GINC-GADI-CPU-CLX-0284\FOpt\RM062X\6-31+G(d,p)\C20H16N3O1(1-)\FJR5
02\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafi
ne) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-Ph-PhOMe.a
s\ -1,1\C,-3.504106353,1.4845795903,-1.1633598496\C,-3.6114010574,0.11
00901026,-0.9809246293\C,-2.5392180988,-0.6119240775,-0.443076411\C,-1
.3599248909,0.0291870313,-0.0427790656\C,-1.2934428683,1.4416831304,-0
.1732762103\C,-2.3296243922,2.1493513448,-0.7736585881\N,-0.1188085496
,2.0078628257,0.3815996523\N,-0.2674770961,-0.6913242666,0.4138690749\
C,0.8965796849,-0.0222809906,0.3017317222\N,1.0753760412,1.2691458191,
0.142147309\C,0.0670987922,3.3982894163,0.456259312\C,-0.9152471971,4.
1998931172,1.0724218631\H,-1.8151149315,3.7352389409,1.4645347921\C,-0
.7410552685,5.5666961975,1.2016420616\H,-1.5003675776,6.1780571327,1.6
805462859\C,0.4314987527,6.1822580988,0.7384418063\C,1.4216083121,5.40
12702975,0.1488389431\H,2.3446580436,5.8429975456,-0.2097064175\C,1.23
46441916,4.019539826,0.0055197947\H,2.010990864,3.4185589302,-0.451683
4592\H,-4.5215275624,-0.4105117093,-1.2663999582\H,-2.5976226304,-1.69
14040094,-0.3271416716\H,-2.2510970283,3.2238503547,-0.9043439109\C,2.
1549076149,-0.841302227,0.3133732945\C,2.0972413398,-2.2286123193,0.13
92900096\H,1.1295670774,-2.6960796455,-0.0079601161\C,3.2625520756,-2.
9956882792,0.1521191832\H,3.2003724132,-4.0714880335,0.0141734405\C,4.
5031505018,-2.3858502077,0.3374858924\C,4.5693123286,-1.0023305972,0.5
156222056\H,5.5301531053,-0.5187905706,0.6679382492\C,3.4048241679,-0.
2377341611,0.5083458088\H,3.4524939602,0.8356912237,0.6598968269\H,-4.
3227978786,2.0522735849,-1.5954512667\O,0.5120734741,7.5341005735,0.92
17336081\C,1.6896105594,8.180870936,0.4718207253\H,1.5620324637,9.2386
682422,0.7035198963\H,1.8211060399,8.0587506938,-0.6097617074\H,2.5757
673608,7.7990793298,0.9924946231\H,5.4107942159,-2.9826131909,0.346666
8806\Version=ES64L-G16RevC.01\State=1-A\HF=-1010.9776242\RMSD=1.367e-
09\RMSF=9.692e-06\Dipole=1.6056067,2.7497285,-0.3192726\Quadrupole=4.8
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952748,-1.5587977,-3.336477,2.8612462,-0.7831357,-1.1054772\PG=C01 [X(C20H16N3O1)]\@

H-Ph-PhOMe.cs

1\1\GINC-GADI-CPU-CLX-0284\FOpt\RM062X\6-31+G(d,p)\C20H16N3O1(1+)\FJR502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-Ph-PhOMe.cs\1,1\C,-3.5740315542,1.5761669812,-0.9784235068\C,-3.6525146443,0.150361789,-0.9898761762\C,-2.560138693,-0.6159282136,-0.6993603924\C,-1.331865792,0.0206184862,-0.3647292231\C,-1.2891323603,1.4511968306,-0.2933845108\C,-2.4213809415,2.2313392947,-0.6395519808\N,-0.0947231501,1.9790565277,0.0973199367\N,-0.2358743545,-0.7103985422,-0.1492158326\C,0.8925525392,-0.0683808413,0.1243861178\N,0.9751202151,1.2691619995,0.2882254489\C,0.0835969708,3.3954164196,0.3208752036\C,-0.7633650451,4.0747758382,1.2005305656\H,-1.5662596468,3.5548870417,1.7140189643\C,-0.5397397147,5.4193802999,1.4304212229\H,-1.1672521762,5.9770056078,2.1172962143\C,0.5175942266,6.0832921906,0.7839426877\C,1.3635781828,5.3837681341,-0.0878827676\H,2.1833108793,5.8785922022,-0.5930569203\C,1.147669681,4.0284590534,-0.3098264296\H,1.7935244183,3.4700485239,-0.980238904\H,-4.5924097153,-0.321297821,-1.2563687599\H,-2.5795494879,-1.6997881427,-0.7306630456\H,-2.3680971907,3.3124995949,-0.6523689605\C,2.1469912755,-0.8298442941,0.3010360127\C,2.137034225,-2.2195752682,0.1261258092\H,1.2116307083,-2.723023118,-0.1317911886\C,3.3129364797,-2.9463612246,0.2828433323\H,3.3016975415,-4.0229431954,0.1458876816\C,4.5016469253,-2.2940992077,0.6134337407\C,4.5125835098,-0.9096302619,0.7878283154\H,5.4352778199,-0.3999483552,1.0459624062\C,3.3407132867,-0.1753356571,0.6329616862\H,3.3514110798,0.9004367854,0.7707942928\H,-4.4495596812,2.1538244445,-1.2547111091\O,0.6448604051,7.3914013173,1.0655712269\C,1.702164366,8.1174656181,0.442020356\H,1.6167528641,9.1382779426,0.811583143\H,1.5890764657,8.1089509758,-0.6467221908\H,2.675851626,7.7040258229,0.7227488816\H,5.4178984559,-2.8638055784,0.7348686524\Version=ES64L-G16RevC.01\State=1-A\HF=-1010.6889873\RMSD=7.586e-09\RMSF=6.385e-06\Dipole=-1.9040323,0.7208537,-1.0078351\Quadrupole=14.0372631,12.7861438,-26.823407,6.5403267,5.6822365,0.0208543\PG=C01 [X(C20H16N3O1)]\@

H-Ph-PhOMe.nd

1\1\GINC-GADI-CPU-CLX-1776\FOpt\UM062X\6-31+G(d,p)\C20H16N3O1(2)\FJR502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-Ph-PhOMe.nd\0,2\C,-3.5949939335,1.5780143031,-0.9752146275\C,-3.6583194312,0.1776136817,-1.0470009928\C,-2.5364571774,-0.5832275396,-0.7633334005\C,-1.3280190808,0.0328950315,-0.3903156542\C,-1.2900442438,1.4466309254,-0.2885381592\C,-2.4206192147,2.2161709309,-0.6021379177\N,-0.078681289,1.9969846989,0.1102558495\N,-0.213294434,-0.7324946022,-0.156394141\C,0.9052632191,-0.0678358815,0.1201932254\N,1.0384616293,1.2519550808,0.2609987113\C,0.1034124537,3.398094127,0.3320648116\C,-0.6700642351,4.0654765219,1.2863162004\H,-1.4220718471,3.5236730559,1.8524843651\C,-0.4643529647,5.4171366604,1.5116099763\H,-1.0505130708,5.9543200181,2.2502009559\C,0.5234156511,6.1096142757,0.7955014123\C,1.3048144841,5.4362800207,-0.1488788234\H,2.0753746963,5.9512257352,-0.7095624384\C,1.0874274693,4.0774457875,-0.3763484129\H,1.6883299765,3.5426701305,-1.1054455625\H,-4.5847996947,-0.308246408,-1.3358595778\H,-2.5529669772,-1.6668249826,-0.8296630982\H,-2.3763859269,3.2981632262,-0.5584352727\C,2.1584817896,-0.856436393,0.3102738941\C,2.151067947,-2.2377629487,0.0844850322\H,1.2305409604,-2.7190533327,-0.2271780426\C,3.3142109386,-2.9850946061,0.2575502547\H,3.296533693,-4.0559804041,0.0785348577\C,4.4963990091,-2.3616494272,0.6572669287\C,4.5087011941,-0.9844675548,0.8835832397\H,5.4244686347,-0.4923006817,1.1970769916\C,3.3478556228,-0.2345016712,0.711698771\H,3.3582758505,0.8351056424,0.8913445597\H,-4.4688579946,2.174506319,-1.2167242192\O,0.6518449665,7.4258047747,1.088313231\C,1.6434382571,8.1682573973,0.3903322285\H,1.5798991087,9.1857694848,0.7748773061\H,1.4457355516,8.1713116555,-0.6870585987\H,2.6435923565,7.7656610118,0.5832357043\H,5.4024760556,-2.9448540636,0.79240043

2\\Version=ES64L-G16RevC.01\\State=2-A\\HF=-1010.8595901\\S2=0.768047\\S2-1=0.\\S2A=0.750192\\RMSD=6.630e-09\\RMSF=6.077e-06\\Dipole=-0.1279451,2.0137614,-0.4792232\\Quadrupole=6.5238955,6.7853328,-13.3092283,4.3027459,1.1320746,-2.5551934\\PG=C01 [X(C20H16N3O1)]\\@

3-(4-chlorophenyl) radical

H-PhCl-Ph.as

1\\1\\GINC-GADI-CPU-CLX-1776\\FOpt\\RM062X\\6-31+G(d,p)\\C19H13Cl1N3(1-)\\FJR502\\20-Feb-2020\\0\\# M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultra fine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\\H-PhCl-Ph.as\\-1,1\\C,-3.5944249258,1.3761533746,-1.18699988\\C,-3.6937107981,0.0314371221,-0.8383193011\\C,-2.5983376878,-0.6308808251,-0.2769291313\\C,-1.3977114879,0.0447375065,-0.0171378014\\C,-1.341632479,1.4324514504,-0.3025460459\\C,-2.4042491515,2.0726944062,-0.9343756446\\N,-0.1337486926,2.0510049768,0.0910170797\\N,-0.2783279828,-0.6307934848,0.4420390474\\C,0.8734602654,0.0217233308,0.209111913\\N,1.0472399125,1.2890233786,-0.099637053\\C,0.0394443705,3.4055487907,0.3109638991\\C,-1.0177755083,4.2106792312,0.7941988452\\H,-1.9874421789,3.7668858312,0.9905490908\\C,-0.8186145293,5.560507489,1.0525115053\\H,-1.6503217831,6.1487270147,1.4313033194\\C,0.4283480567,6.1614936815,0.8492536578\\C,1.4789353351,5.3674694376,0.3918806007\\H,2.4609833383,5.8058085205,0.2332744818\\C,1.3004431552,4.0108977364,0.1263192541\\H,2.1272041111,3.4071354743,-0.2240608718\\H,-4.6175705888,-0.5121800392,-1.0161401968\\H,-2.6508077763,-1.6898300026,-0.0369822418\\H,-2.3248581145,3.1221963854,-1.1991827859\\C,2.1320246063,-0.7943707944,0.2508551333\\C,2.067476072,-2.1910622404,0.2717031436\\H,1.0958025368,-2.6717390147,0.2492153107\\C,3.227212105,-2.963068524,0.315406429\\H,3.1720745612,-4.0467330298,0.3297458354\\C,4.4601085666,-2.321223438,0.3353267386\\C,4.5577320949,-0.9326776617,0.3178312203\\H,5.5296384619,-0.4506298684,0.3403446728\\C,3.3890800779,-0.1777136471,0.2798402584\\H,3.447405017,0.9055081958,0.2777320499\\H,-4.4321835528,1.8930245009,-1.645158524\\Cl,5.9271321372,-3.2813432849,0.3883816023\\H,0.5752624561,7.2174380199,1.0523743886\\Version=ES64L-G16RevC.01\\State=1-A\\HF=-1356.0678465\\RMSD=7.322e-09\\RMSF=4.897e-06\\Dipole=0.7733607,0.5641174,-0.1059932\\Quadrupole=-1.7763831,-0.6811536,2.4575367,7.389888,-0.4669664,1.2703169\\PG=C01 [X(C19H13Cl1N3)]\\@

H-PhCl-Ph.cs

1\\1\\GINC-GADI-CPU-CLX-1788\\FOpt\\RM062X\\6-31+G(d,p)\\C19H13Cl1N3(1+)\\FJR502\\20-Feb-2020\\0\\# M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultra fine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\\H-PhCl-Ph.cs\\1,1\\C,-3.6142288994,1.5508807789,-0.9667580086\\C,-3.6774080125,0.1238334556,-1.0119027136\\C,-2.5763815715,-0.6391968139,-0.7483442396\\C,-1.3513219533,0.0024997503,-0.4112435761\\C,-1.3186007838,1.434621321,-0.3250377126\\C,-2.4645201831,2.2122123092,-0.6314512879\\N,-0.1233610361,1.9646731793,0.0480405467\\N,-0.2506219754,-0.7198917441,-0.1990965929\\C,0.872222555,-0.0732834425,0.0885233152\\N,0.9516598916,1.2652520166,0.2390478866\\C,0.0511035639,3.3927648117,0.2610533864\\C,-0.6937701707,4.0224575947,1.2524446368\\H,-1.4047233105,3.4609954532,1.8515126055\\C,-0.4814478992,5.3825688891,1.4632964534\\H,-1.0425645434,5.8967986628,2.2362157044\\C,0.4511917011,6.0757971755,0.6905311748\\C,1.1874729664,5.4150491564,-0.2937536047\\H,1.9126733209,5.9567782211,-0.8917283458\\C,0.9970976952,4.0534633337,-0.5138994851\\H,1.5586102048,3.5148202016,-1.2707678329\\H,-4.6163326891,-0.3502569016,-1.2769410031\\H,-2.5873583559,-1.7226585912,-0.7974428302\\H,-2.422331875,3.2941688305,-0.6153271544\\C,2.1242296163,-0.8300137166,0.2913679696\\C,2.1100304998,-2.2258830085,0.1875754371\\H,1.1846579577,-2.7432324293,-0.0402442968\\C,3.2774005853,-2.9554428894,0.3774757332\\H,3.2707138321,-4.0373299044,0.3001644699\\C,4.4569864366,-2.275190701,0.6698374602\\C,4.4937679007,-0.8871366612,0.7752987595\\H,5.4239852078,-0.3783465283,1.0029318799\\C,3.3213215527,-0.1654960729,0.585755431\\H,3.3429529843,0.9155586744,0.6691152266\\H,-4.5018181478,2.1239694894,-1.2128905192\\Cl,5.9257204643,-3.18380633,0.9112406455\\H,0.6082824703,7.1363024297,0.859110481\\Version=ES64L-G16RevC.01\\State=1-A\\HF=-1355.7715097\\RMSD=5.006e-09\\RMSF=4.313e-06\\Dipole=-4.3366746,2.6362127,-0.8271637\\Quadrupole=11.5537296,9.32174,-20.8

754696,0.3188997,4.5778013,3.4237434\PG=C01 [X(C19H13C11N3)]\@

H-PhCl-Ph.nd

1\1\GINC-GADI-CPU-CLX-1788\FOpt\UM062X\6-31+G(d,p)\C19H13C11N3(2)\FJR502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-PhCl-Ph.nd\0,2\C,-3.6524473015,1.5161403866,-0.9703148648\C,-3.7057786387,0.1136032128,-1.0001354208\C,-2.5744927729,-0.6299267746,-0.7102366388\C,-1.3669107508,0.0065812614,-0.369950104\C,-1.3397173191,1.422861052,-0.3057664395\C,-2.4795072715,2.1741534799,-0.6297512071\N,-0.1271108584,1.9922984119,0.0649677021\N,-0.2418724312,-0.7432034703,-0.1349066854\C,0.8741213648,-0.0615930765,0.1047282624\N,0.998963751,1.2615330753,0.2119253302\C,0.0477211555,3.3981473365,0.2663365148\C,-0.7453703846,4.0705364931,1.1959094978\H,-1.5001028382,3.5294457219,1.7589956454\C,-0.5453688727,5.4346760266,1.3969176436\H,-1.1567271089,5.9635931159,2.1213113217\C,0.4434363825,6.1133007729,0.6834404493\C,1.2384380426,5.4251989383,-0.2341856023\H,2.0103031648,5.9494615007,-0.788849003\C,1.043980566,4.0623541884,-0.4477793764\H,1.6529023688,3.5102533476,-1.1567918469\H,-4.6318253694,-0.3872704633,-1.2632377659\H,-2.5823453247,-1.7150090278,-0.7467860606\H,-2.4443142921,3.2572841072,-0.6204053526\C,2.1367160965,-0.8337351559,0.2919401405\C,2.1227214906,-2.2277770351,0.1787731172\H,1.1913103675,-2.7357936087,-0.044565546\C,3.2898255678,-2.9669623179,0.3495714331\H,3.2770954327,-4.0483026297,0.2618788189\C,4.4749224881,-2.2966282221,0.6345895426\C,4.5167791712,-0.9103961597,0.7518469594\H,5.4509876582,-0.4063323162,0.9752424415\C,3.3427862836,-0.1840118965,0.5797486918\H,3.3646325812,0.896181074,0.6719466341\H,-4.5334694047,2.0986254873,-1.2196179032\C1,5.9475865666,-3.216508091,0.851129388\H,0.5974180465,7.175521255,0.8457902828\Version=ES64L-G16RevC.01\State=2-A\HF=-1355.9453765\S2=0.76822\S2-1=0.\S2A=0.750194\RMSD=2.758e-09\RMSF=3.030e-06\Dipole=-1.6122544,2.1992653,-0.2143885\Quadrupole=0.7883213,7.6330217,-8.421343,3.8239585,-0.7581404,2.8610189\PG=C01 [X(C19H13C11N3)]\@

3-(4-methylphenyl) radical

H-PhMe-Ph.as

1\1\GINC-GADI-CPU-CLX-1990\FOpt\RM062X\6-31+G(d,p)\C20H16N3(1-)\FJR502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-PhMe-Ph.as\ -1,1\C,-3.5976252658,1.3740185235,-1.2278945084\C,-3.7017694153,0.0386190444,-0.8447286837\C,-2.6132913419,-0.6103028486,-0.2554164897\C,-1.413224961,0.0702647877,-0.0021803397\C,-1.3541139033,1.4506197743,-0.3217247349\C,-2.4094475384,2.0755697492,-0.9808252727\N,-0.1498296001,2.0766417227,0.0672775177\N,-0.2995927304,-0.5932808548,0.4834125383\C,0.8575723851,0.0493793535,0.2419653434\N,1.0327824912,1.3096476469,-0.0974940425\C,0.0204125111,3.4283559937,0.2942309852\C,-1.0484488204,4.2427684526,0.7368013516\H,-2.0284783293,3.8077626953,0.8970628395\C,-0.8484302673,5.5911491054,1.002342975\H,-1.6897808124,6.1852888056,1.3495281277\C,0.4090807353,6.1837534778,0.8454060863\C,1.4700036287,5.3813235602,0.42746237\H,2.4605838376,5.8121919717,0.305344065\C,1.2920640529,4.0262144036,0.1561530185\H,2.1269558144,3.4161518087,-0.1622140107\H,-4.6246894397,-0.5082908395,-1.0176385432\H,-2.6694976956,-1.662483238,0.0119315278\H,-2.3254307973,3.1178116203,-1.2720672899\C,2.1137444762,-0.7677882978,0.3099537739\C,2.0544885693,-2.1632781544,0.3408635533\H,1.0840295008,-2.6469619099,0.308637617\C,3.2219531737,-2.9256373626,0.4067699205\H,3.1524711409,-4.0108329656,0.4282172502\C,4.4800320061,-2.319241122,0.4411866469\C,4.5347143942,-0.9183800658,0.4125502305\H,5.5027290093,-0.4225537842,0.4447812534\C,3.3742418212,-0.1546301759,0.3516955368\H,3.4323980613,0.9291358879,0.3410354157\H,-4.4300926166,1.8792000758,-1.70822388\H,0.5558846347,7.2387597198,1.0534545696\C,5.7460716904,-3.1341112767,0.5105428473\H,5.5258505973,-4.2045299828,0.5295122495\H,6.3892972416,-2.9334478084,-0.3528065979\H,6.3216217611,-2.8885174936,1.4092947828\Version=ES64L-G16RevC.01\State=1-A\HF=-935.7959324\RMSD=5.398e-09\RMSF=5.771e-06\Dipole=1.4213156,0.1707617,-0.0648016\Quadrupole=6.1924899,-1.631506,-4.5609839,-4.3853844,0.497000

5,0.7401705\PG=C01 [X(C20H16N3)]\@

H-PhMe-Ph.cs

1\1\GINC-GADI-CPU-CLX-1990\FOpt\RM062X\6-31+G(d,p)\C20H16N3(1+)\FJR502
\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine)
e) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-PhMe-Ph.cs\
1,1\C,-3.6387179302,1.5664187997,-0.9478926613\C,-3.7037376836,0.13914
98981,-0.986187029\C,-2.6019848808,-0.6238008075,-0.7260493769\C,-1.37
31970451,0.0170541197,-0.3986258154\C,-1.3390589812,1.4487183501,-0.31
89960633\C,-2.4857351036,2.2267761952,-0.6228370379\N,-0.1406140199,1.
9783243382,0.0433290263\N,-0.2734693952,-0.7067308247,-0.1891971667\C,
0.8556747733,-0.0621658649,0.0855660004\N,0.9351654047,1.2790793103,0.
2291189041\C,0.0371002363,3.4068924585,0.2488069539\C,-0.7069776268,4.
0457903935,1.2349262608\H,-1.4202531864,3.4910386052,1.8372762764\C,-0
.4916057473,5.4069573853,1.4363104923\H,-1.0526414119,5.927891601,2.20
48641145\C,0.4436393229,6.0925296086,0.6599393682\C,1.1802398985,5.422
6294212,-0.3178981464\H,1.9080120262,5.9581527846,-0.9183266542\C,0.98
65161795,4.0600475209,-0.5285400991\H,1.5486083029,3.5143813773,-1.279
9148541\H,-4.644641404,-0.3353355018,-1.2435356876\H,-2.6146994362,-1.
7074719643,-0.7705823627\H,-2.4410317058,3.3088138614,-0.6125730906\C,
2.1066423134,-0.8176343724,0.2789151303\C,2.1026784495,-2.2101759118,0
.1418091222\H,1.1807353986,-2.7256473175,-0.1052655968\C,3.2784390541,
-2.9312843205,0.3221352911\H,3.2643301318,-4.0121726837,0.2133324812\C
,4.4790892498,-2.2878443387,0.6416633976\C,4.4704698102,-0.891833603,0
.7756547388\H,5.3934809158,-0.374320606,1.0241042144\C,3.3043588448,-0
.1601516218,0.5981324409\H,3.3216028212,0.9188974218,0.7092946828\H,-4
.5268038553,2.1397436729,-1.1915782365\H,0.6025015864,7.1539767775,0.8
210460825\C,5.7525192271,-3.0634473321,0.8393298632\H,5.589687704,-4.1
339350564,0.6962209928\H,6.520525573,-2.7329704226,0.1325862935\H,6.14
83921892,-2.9059813513,1.8478377505\Version=ES64L-G16RevC.01\State=1-
A\HF=-935.5036214\RMSD=6.168e-09\RMSF=5.551e-06\Dipole=-2.6625019,1.56
62475,-0.5418184\Quadrupole=16.7186039,8.8475448,-25.5661487,-8.319291
9,5.7034266,2.1647875\PG=C01 [X(C20H16N3)]\@

H-PhMe-Ph.nd

1\1\GINC-GADI-CPU-CLX-2000\FOpt\UM062X\6-31+G(d,p)\C20H16N3(2)\FJR502\
20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine)
) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-PhMe-Ph.nd\
2\C,-3.679347256,1.5325413264,-0.9475440509\C,-3.7342136202,0.1298209
928,-0.9695517898\C,-2.6022205172,-0.6130198413,-0.6808731997\C,-1.391
679681,0.0236116489,-0.3496128214\C,-1.363174891,1.4400885347,-0.29254
75141\C,-2.5039861185,2.1906680075,-0.6158260932\N,-0.1480269317,2.008
9367366,0.0690615482\N,-0.2673837192,-0.7265056276,-0.1162955392\C,0.8
541096328,-0.0475137138,0.1110844836\N,0.979444531,1.2775622563,0.2097
150821\C,0.0324374322,3.4158000511,0.2548466541\C,-0.7616255707,4.1046
628172,1.1716029406\H,-1.5217562321,3.5749476561,1.7381754053\C,-0.555
2420707,5.4702299567,1.3564584739\H,-1.167389218,6.0113517391,2.071143
5738\C,0.4407848553,6.1347888782,0.6397978469\C,1.2367003528,5.4307230
819,-0.2648141207\H,2.0143996154,5.9436215102,-0.8220013642\C,1.035902
1156,4.0664543311,-0.4622132091\H,1.6455749209,3.5021386921,-1.1607893
842\H,-4.6618781228,-0.3718090151,-1.2257122878\H,-2.61105956,-1.69829
71498,-0.7117748868\H,-2.4678554254,3.2737464262,-0.6123719291\C,2.116
3147892,-0.8198399745,0.2898997304\C,2.1192618172,-2.2061809175,0.1124
593581\H,1.1969052392,-2.7102856985,-0.1552161647\C,3.2950413853,-2.93
68154061,0.2749572827\H,3.2789013591,-4.0141827212,0.1309542689\C,4.49
51996048,-2.3081925334,0.6186135741\C,4.4836365786,-0.9175468759,0.794
9411139\H,5.4053319201,-0.4068848401,1.0643328734\C,3.316052078,-0.180
9778185,0.6337362255\H,3.3285053823,0.8941952144,0.7776250048\H,-4.560
7931367,2.1147605807,-1.1960352371\H,0.5996120194,7.198123994,0.789845
0188\C,5.7690453961,-3.0912646714,0.7982129309\H,5.6065428758,-4.15653
66088,0.6173531648\H,6.5435201246,-2.7403444062,0.1083505178\H,6.15964
80454,-2.9722166125,1.8142125195\Version=ES64L-G16RevC.01\State=2-A\H
F=-935.6751984\S2=0.768183\S2-1=0.\S2A=0.750195\RMSD=3.392e-09\RMSF=4.
551e-06\Dipole=-0.4505359,1.5027713,-0.0526554\Quadrupole=7.5807849,6.

4063262,-13.98711111,-6.1554853,0.9990791,1.59047\PG=C01 [X(C20H16N3)]\@

3-(4-nitrophenyl) radical

H-PhNO2-Tri.as

1\1\GINC-GADI-CPU-CLX-2000\FOpt\RM062X\6-31+G(d,p)\C19H13N4O2(1-)\FJR502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-PhNO2-Tri.as\ -1,1\C,-3.6000887761,1.3070005794,-0.9497017448\C,-3.626479363,-0.035368648,-0.5819439746\C,-2.47025581,-0.6516762167,-0.0940238241\C,-1.280433351,0.0691302598,0.0727276185\C,-1.2938325248,1.4541315736,-0.2292930685\C,-2.4203943319,2.0484337559,-0.7897182706\N,-0.0833142071,2.1219919538,0.0732853634\N,-0.1060418241,-0.5626850003,0.4538688958\C,0.9986511102,0.1316030431,0.1356942384\N,1.1064588005,1.4011149546,-0.1887884229\C,0.0539407558,3.494145775,0.2160108312\C,-0.9839484291,4.2737374497,0.7739591161\H,-1.9068396174,3.7975570655,1.0866505181\C,-0.8222834838,5.6410252702,0.9552971544\H,-1.6367631159,6.2112978513,1.393965922\C,0.3693395916,6.2821410638,0.599943152\H,0.4880071098,7.3512508284,0.7442188795\C,1.4033811826,5.5133380346,0.0685479525\H,2.3429764942,5.9845982469,-0.2082137226\C,1.2603330655,4.1397393468,-0.122515331\H,2.0736780422,3.5553814517,-0.5325454988\C,2.2878997575,-0.6353214468,0.0917494467\C,2.2737277081,-2.0324169622,0.1864903025\H,1.3214198743,-2.5406454872,0.2815931685\C,3.4576611002,-2.7603566364,0.1546999027\H,3.454804867,-3.8415210525,0.225846595\C,4.656257714,-2.0675823253,0.0225193793\C,4.7086330744,-0.6789418143,-0.0717503516\H,5.6614688045,-0.1722683083,-0.1682283065\C,3.5163857871,0.0306448458,-0.0304653704\H,3.5280075465,1.1130067193,-0.0887708188\H,-4.4861928566,1.7890401954,-1.351328224\H,-4.5404170797,-0.6133294616,-0.6876288061\H,-2.4664657405,-1.7089464625,0.1586144215\H,-2.3988762716,3.0967189306,-1.0693391583\N,5.9089252893,-2.8245492112,-0.0169726051\O,5.8530421043,-4.0415236091,0.0803447541\O,6.9544870031,-2.2049565528,-0.1459501138\Version=ES64L-G16RevC.01\State=1-A\HF=-1100.9364391\RMSD=7.255e-09\RMSF=8.313e-06\Dipole=-0.3424735,1.3142765,-0.1742516\Quadrupole=-13.5399453,-0.0509785,13.5909238,20.411952,0.0821656,0.483297\PG=C01 [X(C19H13N4O2)]\@

H-PhNO2-Tri.cs

1\1\GINC-GADI-CPU-CLX-0266\FOpt\RM062X\6-31+G(d,p)\C19H13N4O2(1+)\FJR502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-PhNO2-Tri.cs\ 1,1\C,-3.6349198999,1.4724554039,-0.6717927165\C,-3.6492880228,0.0436463321,-0.6744306346\C,-2.4992939186,-0.6726611159,-0.5048824098\C,-1.2729463772,0.0218528394,-0.3097793152\C,-1.2844842314,1.4569420723,-0.2631353887\C,-2.4832674555,2.1841543132,-0.4714596705\N,-0.0784228569,2.0397467733,-0.026504403\N,-0.1295786667,-0.6546473165,-0.190400645\C,0.9877028802,0.0405635766,-0.0311010091\N,1.0352858394,1.3823955633,0.0743275201\C,0.0639669737,3.4788722596,0.128375598\C,-0.6027110624,4.1134749615,1.1710744484\H,-1.2306162809,3.5474987379,1.8529867882\C,-0.4199582838,5.4856391315,1.3224319268\H,-0.9205175928,6.0045356381,2.1328926202\C,0.4067606346,6.1852893461,0.4423049875\H,0.5412207364,7.2550757665,0.5653932117\C,1.0662793524,5.5195367436,-0.5918105329\H,1.7089736373,6.0664980068,-1.2735021883\C,0.9048699341,4.1462417386,-0.7545973988\H,1.4079743441,3.6036997447,-1.5488501121\C,2.2837125824,-0.671545545,0.0693280312\C,2.30419886,-2.0671609767,-0.0359355907\H,1.3809493186,-2.6137264295,-0.1886479644\C,3.5072102579,-2.7547330088,0.0560951199\H,3.5430752472,-3.8344476267,-0.0225157792\C,4.6706986059,-2.0210949859,0.2525310886\C,4.6816896399,-0.6357748435,0.3604912388\H,5.611940192,-0.1026758937,0.5144496445\C,3.4726281889,0.0417558879,0.2670106083\H,3.4578080148,1.1223494882,0.3507387558\H,-4.5638047608,2.006808895,-0.8407681066\H,-4.5917648838,-0.4700495002,-0.8306704674\H,-2.4741724453,-1.7567607871,-0.524896912\H,-2.4819716512,3.2668719666,-0.4866868545\N,5.9492612372,-2.7450890518,0.3514783602\O,5.9251665639,-3.9602342541,0.256439047\O,6.9632053492,-2.0903638514,0.5228691039\Version=ES64L-G16RevC.01\State=1-A\HF=-1100.6351174\RMSD=6.430e-09\RMSF=

6.719e-06\Dipole=-6.3563374,3.5564173,-0.6036267\Quadrupole=3.989692,8.85952,-12.849212,11.1146352,0.0758737,3.3585251\PG=C01 [X(C19H13N4O2)]\@

H-PhNO2-Tri.nd

1\1\GINC-GADI-CPU-CLX-0266\FOpt\UM062X\6-31+G(d,p)\C19H13N4O2(2)\FJR502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-PhNO2-Tri.nd\0,2\C,-3.6677668226,1.4451393876,-0.6860938129\C,-3.6742276878,0.0415163329,-0.6788246951\C,-2.4949510578,-0.6566334458,-0.4821137476\C,-1.2845902841,0.0288190363,-0.274167694\C,-1.3010356335,1.4465761988,-0.2454596899\C,-2.4918852452,2.1509081529,-0.4748597559\N,-0.0791571527,2.066854425,-0.0063670172\N,-0.1158042444,-0.6766153783,-0.1308697444\C,0.9900438872,0.0509513009,-0.0120006596\N,1.0792110062,1.3777987826,0.0526713356\C,0.0629853836,3.4835548115,0.1415723174\C,-0.6558949794,4.1528131924,1.1315625181\H,-1.3277887247,3.6012098535,1.7825296224\C,-0.4886444202,5.5283030001,1.2771370317\H,-1.042376853,6.0556590302,2.0474886524\C,0.3950012528,6.220841512,0.4483631802\H,0.5238961401,7.2920646028,0.5674831088\C,1.117446783,5.5359109245,-0.529611977\H,1.807356978,6.0714962489,-1.1741114803\C,0.9543713326,4.1614787597,-0.6884371661\H,1.5074946075,3.6115608313,-1.4434238772\C,2.2927931054,-0.6745820488,0.0743734942\C,2.3101643013,-2.0717804162,-0.0109468746\H,1.3782846401,-2.6099172605,-0.137949306\C,3.510037609,-2.7682344786,0.0658182708\H,3.5361663152,-3.8493386969,0.0009705767\C,4.6846382951,-2.0428845446,0.2277532003\C,4.7022814243,-0.6548774273,0.3158776417\H,5.6383271001,-0.1245945992,0.4430092841\C,3.4947147323,0.0266637245,0.2379896554\H,3.4828880254,1.108149483,0.3065535994\H,-4.5887412259,1.9913056013,-0.8624437961\H,-4.6028983074,-0.4961549729,-0.8401674773\H,-2.4676313416,-1.741919267,-0.4927143303\H,-2.4947941608,3.2344565521,-0.4931405051\N,5.9570135794,-2.7707454385,0.3092675682\O,5.9283070119,-3.9887232441,0.2332427981\O,6.9816246305,-2.1220905262,0.448889751\Version=ES64L-G16RevC.01\State=2-A\HF=-1100.8117893\S2=0.768702\S2-1=0.\S2A=0.7502\RMSD=5.847e-09\RMSF=3.197e-06\Dipole=-3.1640686,2.9763813,-0.209852\Quadrupole=-9.4910622,7.9681332,1.522929,15.1789411,-3.0028811,2.5857276\PG=C01 [X(C19H13N4O2)]\@

3-(4-methoxyphenyl) radical

H-PhOMe-Ph.as

1\1\GINC-GADI-CPU-CLX-0266\FOpt\RM062X\6-31+G(d,p)\C20H16N3O1(1-)\FJR502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-PhOMe-Ph.as\-1,1\C,-3.5925009893,1.3174738828,-1.1632910129\C,-3.6626252357,-0.0073828342,-0.7380759638\C,-2.5510157351,-0.6153462215,-0.1485861395\C,-1.3608680722,0.0963789387,0.0622441318\C,-1.3348664043,1.4669143702,-0.3013834813\C,-2.4148834543,2.0499586083,-0.9593813861\N,-0.1365963623,2.1278012189,0.0470962274\N,-0.2264796054,-0.5291199069,0.5513831054\C,0.9139473959,0.1271653079,0.2686223674\N,1.0581201331,1.3776254065,-0.1206758151\C,0.0125449909,3.4930860204,0.1988946778\C,-1.0581698603,4.3047423952,0.6414323895\H,-2.0203395551,3.8555103662,0.8608798515\C,-0.8818421346,5.6688981537,0.8312066768\H,-1.723456976,6.2613267379,1.1805789919\C,0.3546375066,6.2802911795,0.59665759\C,1.4182782875,5.4815801297,0.1789178361\H,2.3926884047,5.9280230789,-0.0028720941\C,1.2634311473,4.1104286735,-0.0174187551\H,2.1000363996,3.5034707388,-0.3376346122\H,-4.5767280631,-0.5780598196,-0.8777008657\H,-2.5813016279,-1.6595501879,0.152558993\H,-2.3578770626,3.0843691015,-1.2830746292\C,2.184150811,-0.6621194733,0.3484953123\C,2.1573165315,-2.0642160517,0.3302423042\H,1.1996111104,-2.5677850237,0.2526965587\C,3.3287619829,-2.8043910087,0.4055156127\H,3.3091030542,-3.8900775206,0.3883176776\C,4.5655269592,-2.1540113834,0.5014585141\C,4.6136623259,-0.7569712599,0.5252969645\H,5.5569459656,-0.2296963441,0.6082065574\C,3.424818855,-0.0293508595,0.4519047299\H,3.4617356028,1.0550021765,0.482646166\H,-4.4434365813,1.7909995954,-1.6435764288\O,5.66034985,-2.9581476252,0.5706783379\C,6.932041754,-2.335353613,0.6675516644\H,7.6607715264,-3.1450940088,0.7071229848\H,7.0082703061,-1.7318311675,1.5789621879\H,7.13239

07934,-1.7070470787,-0.2076009453\H,0.4835460255,7.3475253077,0.745853
7181\Version=ES64L-G16RevC.01\State=1-A\HF=-1010.9808151\RMSD=4.059e-
09\RMSF=8.275e-06\Dipole=2.3968552,0.4422892,-0.0042019\Quadrupole=13.
2779984,-8.9109518,-4.3670465,-1.0726297,1.3867222,1.4126517\PG=C01 [X
(C20H16N3O1)]\@

H-PhOMe-Ph.cs

1\1\GINC-GADI-CPU-CLX-0266\FOpt\RM062X\6-31+G(d,p)\C20H16N3O1(1+)\FJR5
02\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafi
ne) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-PhOMe-Ph.c
s\1,1\C,-3.6357964717,1.5181380677,-0.8792132604\C,-3.6749014237,0.08
93944902,-0.8617457025\C,-2.5528707332,-0.643516685,-0.6025969614\C,-1
.3271405246,0.0305189676,-0.3341183557\C,-1.3182235943,1.464327588,-0.
3090012222\C,-2.4873308722,2.2103448348,-0.6096619315\N,-0.1202834224,
2.0279732963,0.0016070868\N,-0.208867061,-0.665375723,-0.1295476867\C,
0.9160885114,0.0081365253,0.0928186677\N,0.9725815113,1.3567547617,0.1
859523565\C,0.0354378176,3.4670318502,0.147738764\C,-0.6861819537,4.12
56383691,1.1374692535\H,-1.3660032841,3.578125235,1.7837970542\C,-0.49
29989094,5.4970192329,1.2834248109\H,-1.0363880575,6.0337468818,2.0537
477486\C,0.3985722921,6.173045661,0.4494165418\C,1.1121654255,5.483900
4459,-0.5321414524\H,1.805107414,6.0124905018,-1.1781806735\C,0.940373
8633,4.1108734631,-0.6878952794\H,1.4847843587,3.5503480646,-1.4413579
16\H,-4.6133846358,-0.4113318913,-1.0749162107\H,-2.547710896,-1.72802
56109,-0.6051469349\H,-2.4648020328,3.2925280784,-0.6381649984\C,2.180
6340381,-0.7156752895,0.2774648771\C,2.2006839582,-2.1188042648,0.1897
54054\H,1.2821066017,-2.6590460972,-0.0120702025\C,3.3822789775,-2.813
9926451,0.3594449171\H,3.4099673621,-3.8968942136,0.2939713989\C,4.576
5840572,-2.1214822502,0.6212930138\C,4.5692674824,-0.7233397928,0.7108
631964\H,5.4778933375,-0.169647878,0.9130117202\C,3.374222176,-0.03337
51447,0.5383337505\H,3.3770047287,1.0490446336,0.6111080257\H,-4.54088
21174,2.0658638661,-1.1192919316\O,5.6768309641,-2.8834192721,0.772072
2839\C,6.9161954232,-2.233853966,1.038821242\H,7.6556467326,-3.0293266
882,1.1215958045\H,6.8693446837,-1.6756000562,1.9795145516\H,7.1887626
852,-1.5619074814,0.2184605352\H,0.5409315878,7.242390135,0.5675190648
\Version=ES64L-G16RevC.01\State=1-A\HF=-1010.6895057\RMSD=2.245e-09\R
MSF=6.634e-06\Dipole=-2.6711086,2.2603777,-0.4713367\Quadrupole=27.840
4021,-0.0210092,-27.8193929,-7.4689428,7.2684468,0.8552715\PG=C01 [X(C
20H16N3O1)]\@

H-PhOMe-Ph.nd

1\1\GINC-GADI-CPU-CLX-2721\FOpt\UM062X\6-31+G(d,p)\C20H16N3O1(2)\FJR50
2\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafi
ne) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\H-PhOMe-Ph.nd
\0,2\C,-3.6754803931,1.4854271347,-0.8715362289\C,-3.7035884798,0.082
0798601,-0.8411767803\C,-2.549220784,-0.6291525661,-0.5614648487\C,-1.
341233649,0.0408685489,-0.2925506086\C,-1.3385902048,1.4586242135,-0.2
885754473\C,-2.5033126157,2.1764785611,-0.6013852432\N,-0.1242866803,2
.0624090584,0.0130434177\N,-0.195883167,-0.678788026,-0.0655042121\C,0
.9190286086,0.0274851438,0.1025652776\N,1.0219435468,1.3589862671,0.14
63279507\C,0.029783554,3.4783288121,0.1484844204\C,-0.7390262646,4.173
4638159,1.0817934015\H,-1.4576726124,3.641014948,1.6977354088\C,-0.561
5965264,5.5486337719,1.2179040528\H,-1.1546451639,6.0948631493,1.94463
41347\C,0.3814802533,6.2167501868,0.4359481523\C,1.1533014062,5.506825
3647,-0.4848485599\H,1.8894329635,6.0231191929,-1.0929762833\C,0.98069
53809,4.1323837713,-0.6335588317\H,1.5722882494,3.5635385807,-1.343934
023\H,-4.6289996434,-0.4453611114,-1.0491504198\H,-2.5388085927,-1.714
8338925,-0.5518554469\H,-2.4879303945,3.2595032048,-0.6374037049\C,2.1
963080632,-0.7154078163,0.274693769\C,2.2175685957,-2.1138614565,0.157
4213639\H,1.2959496623,-2.6426503926,-0.0601208911\C,3.3978660115,-2.8
215015858,0.3156049318\H,3.4188784245,-3.9031205504,0.2247433586\C,4.5
928326956,-2.1438775108,0.5962680331\C,4.5887163781,-0.7502356786,0.71
58701132\H,5.4982009966,-0.203357505,0.9342973162\C,3.3933140981,-0.05
13647135,0.5536305517\H,3.3961683952,1.0291477462,0.6506467731\H,-4.57
55750762,2.0417932389,-1.1123581331\O,5.6964282819,-2.9177220974,0.735

4170355\C, 6.9292181967, -2.2729393156, 1.0263517549\H, 7.6719229382, -3.0671170242, 1.0985203694\H, 6.8761910891, -1.7340893035, 1.9786613498\H, 7.2101156978, -1.5811952159, 0.2247502191\H, 0.5179167606, 7.2878711912, 0.5472365072\Version=ES64L-G16RevC.01\State=2-A\HF=-1010.8603116\S2=0.768058\S2-1=0.\S2A=0.750193\RMSD=4.218e-09\RMSF=5.720e-06\Dipole=-0.0423895, 2.016127, 0.0470829\Quadrupole=15.8912527, -1.2807585, -14.6104943, -4.2251503, 2.5700007, 0.7156205\PG=C01 [X(C20H16N3O1)]\@\@

7-methyl radical

Me-Ph-Ph.as

1\1\GINC-GADI-CPU-CLX-2000\FOpt\RM062X\6-31+G(d,p)\C20H16N3(1-)\FJR502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\Me-Ph-Ph.as\1,1\C, -3.6384747223, 1.247349466, -0.6480847889\C, -3.6136077142, -0.084099244, -0.2368089045\C, -2.4227924961, -0.6850458932, 0.1882467365\C, -1.2270435588, 0.0378230594, 0.2510783457\C, -1.2730071191, 1.4123339928, -0.0953199588\C, -2.441476864, 1.9836950324, -0.589119491\N, -0.0479078236, 2.0908085853, 0.0872835629\N, -0.0240971535, -0.5760255775, 0.5718961143\C, 1.0529107869, 0.1039713156, 0.1467707311\N, 1.1247300228, 1.3611798483, -0.2415150649\C, 0.102943384, 3.4582287418, 0.2242037313\C, -0.9070404317, 4.2557444357, 0.8112058859\H, -1.8256896276, 3.7951494274, 1.1567106653\C, -0.7220969007, 5.6214907334, 0.981485655\H, -1.5155771338, 6.2027579063, 1.4439685445\C, 0.4642812499, 6.2482622581, 0.5854458951\H, 0.59988388, 7.3165227613, 0.7206838364\C, 1.4708241729, 5.4634357518, 0.0243692755\H, 2.4069101772, 5.9215827016, -0.2848854937\C, 1.3063790582, 4.0911725515, -0.1551702787\H, 2.0992380252, 3.4953976085, -0.5879331727\C, 2.3411094488, -0.6601709543, 0.0412098472\C, 2.3346011167, -2.0594146103, 0.0348386701\H, 1.3839619704, -2.5772492957, 0.1029437303\C, 3.5280239996, -2.7749795071, -0.0619143154\H, 3.5057767144, -3.8611088252, -0.0677970601\C, 4.7456003903, -2.1006206427, -0.154726603\H, 5.6753178167, -2.6573178046, -0.2302635482\C, 4.7611897996, -0.7043560317, -0.145957681\H, 5.7050154032, -0.1703802738, -0.2110098243\C, 3.5689591443, 0.0095644126, -0.0452118451\H, 3.5780206816, 1.0946837444, -0.0264253094\H, -4.5298410585, -0.6699877991, -0.2615898073\H, -2.4026785985, -1.735134067, 0.4693761158\H, -2.4429622441, 3.0239412731, -0.9037417585\C, -4.9078079026, 1.9073589511, -1.1278393286\H, -5.7160956733, 1.1770064614, -1.2241009514\H, -5.2417323421, 2.6867171869, -0.4331643969\H, -4.764407878, 2.3835823196, -2.1038777603\Version=ES64L-G16RevC.01\State=1-A\HF=-935.7945624\RMSD=8.203e-09\RMSF=2.192e-06\Dipole=-0.1234396, 0.9478365, -0.4238183\Quadrupole=7.1640367, -2.9715055, -4.1925311, -2.2847767, -0.7990832, 1.9265284\PG=C01 [X(C20H16N3)]\@\@

Me-Ph-Ph.cs

1\1\GINC-GADI-CPU-CLX-2000\FOpt\RM062X\6-31+G(d,p)\C20H16N3(1+)\FJR502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\Me-Ph-Ph.cs\1,1\C, -3.6041673209, 1.4042202336, -0.6122804659\C, -3.5824158115, -0.0352418244, -0.6168902862\C, -2.4299005461, -0.7414279916, -0.4565243404\C, -1.2032826722, -0.0392536994, -0.2657852846\C, -1.2359945616, 1.395999662, -0.2194142764\C, -2.4433092897, 2.1096783225, -0.4152088982\N, -0.0357381859, 1.989251006, 0.0069737084\N, -0.0576848785, -0.7030953759, -0.1520031041\C, 1.0611474623, 0.0028892234, 0.0032464746\N, 1.089775377, 1.343448587, 0.103783364\C, 0.0926894757, 3.4302016696, 0.1528570538\C, -0.555715952, 4.0605159162, 1.2092766487\H, -1.160096067, 3.488517855, 1.9071510019\C, -0.3899760889, 5.4360095165, 1.3509195215\H, -0.877359706, 5.9511257045, 2.1718408552\C, 0.4033823476, 6.1442599446, 0.4472758661\H, 0.5254504902, 7.2163768366, 0.5630222702\C, 1.0453813449, 5.4835391488, -0.6009095161\H, 1.6628034378, 6.0368171667, -1.3006689304\C, 0.8991338362, 4.1071430573, -0.7543280504\H, 1.3900369717, 3.5685384454, -1.5588313159\C, 2.359974646, -0.6967470599, 0.0974571347\C, 2.3993582581, -2.0923696266, -0.0126595618\H, 1.4799615489, -2.6467356112, -0.1661432716\C, 3.6164242241, -2.761101883, 0.0763626058\H, 3.6423578897, -3.8427922158, -0.0092171351\C, 4.797220175, -2.0445794913, 0.2748386058\H, 5.7454062374, -2.5688224008, 0.3445381556\C, 4.7590225115, -0.6538114858, 0.384333384\H, 5.6756067064, -0.093950391, 0.5397923273\C, 3.5460700011, 0.0224253925, 0.2967065456\H, 3.5192932492, 1.1031971992, 0.3

847777554\H,-4.5219865256,-0.5590832262,-0.7690365706\H,-2.3995047852,-1.8253968297,-0.478666107\H,-2.4493560086,3.1932576914,-0.4229971835\C,-4.9117792849,2.099690084,-0.831991428\H,-5.6272453121,1.8034357083,-0.0576774688\H,-4.7962389246,3.1842279259,-0.8122659024\H,-5.3374042694,1.8035128154,-1.7963941815\\Version=ES64L-G16RevC.01\State=1-A\HF=-935.5062383\RMSE=4.391e-09\RMSF=5.858e-06\Dipole=-2.5798193,1.1322839,-0.3077876\Quadrupole=16.3042349,7.4905769,-23.7948118,-2.9214727,1.7046296,2.4818215\PG=C01 [X(C20H16N3)]\@

Me-Ph-Ph.nd

1\1\GINC-GADI-CPU-CLX-0784\FOpt\UM062X\6-31+G(d,p)\C20H16N3(2)\FJR502\21-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\Me-Ph-Ph.nd.nd\0,2\C,-2.9865543905,-2.4753785675,-0.1722231006\C,-2.0524204196,-3.5242325825,-0.0402524017\C,-0.7004607828,-3.263061226,0.0746770095\C,-0.2218043083,-1.939198132,0.0770993195\C,-1.1646285062,-0.8868569716,-0.0149459247\C,-2.5338223627,-1.1614221231,-0.1606629046\N,-0.6427267318,0.3999541021,0.0219903366\N,1.1266036632,-1.6947767896,0.1400997406\C,1.4931522364,-0.4184773898,0.0553705974\N,0.6878667343,0.6421472504,-0.0082251173\C,-1.4585201075,1.5747302443,0.0327896044\C,-2.4107583996,1.7491575153,1.0370143779\H,-2.5368060801,0.9900521223,1.8033015545\C,-3.1821413829,2.9092751354,1.0472782145\H,-3.9226208134,3.0520263663,1.8280269681\C,-2.994329579,3.8874101478,0.0698537606\H,-3.5957562982,4.7909884852,0.0835283753\C,-2.0287796757,3.7064623429,-0.9213379475\H,-1.8780052926,4.4663992968,-1.6816520913\C,-1.2555719627,2.5477188871,-0.9449588645\H,-0.4993471527,2.3904209841,-1.7075704816\C,2.9539264965,-0.1103619343,0.0390032896\C,3.8839612731,-1.155797985,0.004283966\H,3.5292218609,-2.1805371508,-0.0104445364\C,5.2500711238,-0.8819097102,-0.0120500719\H,5.9618664226,-1.7015428312,-0.039765804\C,5.7020095532,0.4376532046,0.0058103072\H,6.7668635535,0.6503677768,-0.0065465345\C,4.7784357259,1.483468952,0.040425503\H,5.1222241322,2.5133179134,0.0565988388\C,3.4122431537,1.2132206516,0.0569483442\H,2.6961131088,2.0273005582,0.0871256265\H,-2.4065946616,-4.5518055368,-0.0425881837\H,0.0264356145,-4.0657435687,0.1552958973\H,-3.2442782744,-0.3493615418,-0.2714217759\C,-4.4512257293,-2.7861370594,-0.3280937791\H,-4.820704735,-3.35234095,0.5332049552\H,-5.0430253427,-1.8725011357,-0.4181459468\H,-4.6250116634,-3.3982287503,-1.2191311207\\Version=ES64L-G16RevC.01\State=2-A\HF=-935.6753012\S2=0.768599\S2-1=0.\S2A=0.750202\RMSE=6.194e-09\RMSF=2.938e-06\Dipole=-1.9503015,0.5200844,-0.1213599\Quadrupole=8.4412807,3.8182794,-12.2595601,1.0522245,-2.7465091,-1.2595097\PG=C01 [X(C20H16N3)]\@

7-methoxy radical

MeO-Ph-Ph.as

1\1\GINC-GADI-CPU-CLX-2729\FOpt\RM062X\6-31+G(d,p)\C20H16N3O1(1-)\FJR502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\MeO-Ph-Ph.as\-1,1\C,-3.5895253976,1.058994011,-0.9126611073\C,-3.581908258,-0.2734233169,-0.4978257459\C,-2.4035474189,-0.8420434639,-0.0159272354\C,-1.2239473311,-0.0958961945,0.1068239186\C,-1.276467341,1.2672639092,-0.2521636607\C,-2.4272300347,1.8316376359,-0.8099080683\N,-0.0735312539,1.9689908728,-0.0271647024\N,-0.0248682726,-0.6883770252,0.4963282695\C,1.0558812437,0.0005640879,0.1053681723\N,1.1230004268,1.2529718828,-0.3078678337\C,0.0461639093,3.3400977124,0.0951663208\C,-0.9984193384,4.1252274034,0.6379487435\H,-1.9173936216,3.6502437582,0.9633867329\C,-0.8461140022,5.4968889566,0.7935293337\H,-1.6648981895,6.0685149125,1.2227643718\C,0.3402267852,6.1415364351,0.4269031676\C,1.3797045952,5.3695714496,-0.0905139651\H,2.3159455841,5.8425024475,-0.3761692757\C,1.2479857281,3.992149485,-0.2561613756\H,2.0653538727,3.4070206407,-0.6564620094\H,-4.496390152,-0.8543912663,-0.5710504773\H,-2.3812957699,-1.8891266338,0.2751226719\H,-2.4144208909,2.866240787,-1.1288171227\C,2.3603993023,-0.7427272186,0.0689030984\C,2.3751322661,-2.1418889953,0.0836830965\H,1.4290596182,-2.6716256978,0.1166298512\C,3.5816607211,-2.8406489657,0.0518900457\H,3.5756375761,-3.9269540006,0.0621697396\C,

4.7922334846,-2.1489887397,0.0023860113\C,4.7866955904,-0.752819189,-0.0106629509\H,5.7245804068,-0.2054788887,-0.0425352599\C,3.5807097277,-0.0556003303,0.0261237312\H,3.5742163389,1.0296425922,0.029104889\H,5.7325248622,-2.6923104894,-0.0230995291\O,-4.7768635644,1.5402500919,-1.3996662278\C,-4.8132582193,2.8947292498,-1.8097480252\H,-5.8326260727,3.081472912,-2.1494731149\H,-4.1165037421,3.0813225497,-2.6355592446\H,-4.5791052849,3.570165193,-0.9774966085\H,0.4508421161,7.2138914395,0.5521813748\\Version=ES64L-G16RevC.01\State=1-A\HF=-1010.9771594\RMSD=4.336e-09\RMSF=9.253e-06\Dipole=-0.3213284,1.6044842,-0.6688126\Quadrupole=2.6584896,0.2578565,-2.9163461,-6.405546,-0.4461444,0.0865955\PG=C01 [X(C20H16N3O1)]\@

MeO-Ph-Ph.cs

1\1\GINC-GADI-CPU-CLX-0788\FOpt\RM062X\6-31+G(d,p)\C20H16N3O1(1+)\FJR502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\\MeO-Ph-Ph.cs\\1,1\C,-3.5537098536,1.1824604779,-0.9564942997\C,-3.5208218321,-0.2602604911,-0.9360852505\C,-2.3674778062,-0.9280476815,-0.6959783279\C,-1.1615378052,-0.1927673741,-0.4515115493\C,-1.2271310752,1.2473342501,-0.4447100352\C,-2.4235638033,1.9391583424,-0.7159649808\N,-0.0504439006,1.8643868234,-0.1689212421\N,-0.0226446719,-0.8308185578,-0.2534569279\C,1.080823204,-0.098523009,-0.0463469038\N,1.0825722774,1.2348438411,0.0130994501\C,0.0530272875,3.3096859183,-0.0668306318\C,-0.6579696049,3.9679315296,0.9309816844\H,-1.2921427263,3.4116242009,1.6150447189\C,-0.5183591317,5.3499436264,1.0326394384\H,-1.0549517533,5.8856969708,1.8085326757\C,0.3135810602,6.038292567,0.1482622637\C,1.0187025475,5.351064895,-0.8404350262\H,1.6666091314,5.8888837651,-1.5245145688\C,0.896821892,3.9681309347,-0.9535985583\H,1.438051532,3.4095667045,-1.7108331001\H,-4.450875766,-0.7842994074,-1.1313029931\H,-2.3135936247,-2.0111071152,-0.6897111909\H,-2.4433954424,3.0197874832,-0.7375535712\C,2.3776660388,-0.7820009337,0.1507899005\C,2.437357158,-2.1798440515,0.0976190133\H,1.5346910484,-2.7517281908,-0.0878290046\C,3.6540679208,-2.8300777125,0.2842775952\H,3.6955177032,-3.9139260191,0.2426652334\C,4.8139551687,-2.092796625,0.5239496175\C,4.7552666464,-0.6991670197,0.5767209874\H,5.6553050811,-0.1221318882,0.7637736213\C,3.5430078931,-0.042039775,0.3916835617\H,3.4993321462,1.0409797502,0.4351974754\H,5.761595973,-2.6020783194,0.6697566187\O,-4.7502551954,1.6876739124,-1.2264356676\C,-4.9044091759,3.1106362488,-1.2681055534\H,-5.9533005065,3.2840556978,-1.4993837965\H,-4.2709087321,3.5372142246,-2.0506784328\H,-4.6566903666,3.5464817057,-0.2958753081\H,0.4158710641,7.1153703008,0.2330430649\\Version=ES64L-G16RevC.01\State=1-A\HF=-1010.6940821\RM SD=3.182e-09\RMSF=4.558e-06\Dipole=-2.2952836,1.5587149,-0.426585\Quadrupole=12.3208646,11.0430208,-23.3638854,-8.6195626,3.2746454,-0.0389021\PG=C01 [X(C20H16N3O1)]\@

MeO-Ph-Ph.nd

1\1\GINC-GADI-CPU-CLX-0682\FOpt\UM062X\6-31+G(d,p)\C20H16N3O1(2)\FJR502\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\\MeO-Ph-Ph.nd\0,2\C,-3.5907195258,1.1532455755,-0.9485836267\C,-3.5598624394,-0.2569301694,-0.9021635901\C,-2.3763593114,-0.9094620271,-0.6348151377\C,-1.1876327314,-0.1915636844,-0.3926665662\C,-1.2476919524,1.2226457381,-0.4116615547\C,-2.4415002305,1.8997604364,-0.7092313382\N,-0.0578827705,1.8817097149,-0.1438205553\N,-0.011986367,-0.8615389021,-0.1718225711\C,1.0735645813,-0.1046246475,-0.0267070373\N,1.1213916995,1.2262693339,-0.0099190886\C,0.0454095159,3.3058130025,-0.0547404129\C,-0.7231428278,4.0013340104,0.8786211698\H,-1.4038462625,3.4617844124,1.5305989217\C,-0.5941238386,5.3858787744,0.968036073\H,-1.1865529599,5.9323474957,1.6951271085\C,0.3021139947,6.0635034136,0.1403796651\C,1.0749231657,5.3540472717,-0.779851946\H,1.7751725968,5.8775892384,-1.4231216003\C,0.9491589517,3.9703333308,-0.882706235\H,1.5425273479,3.4018211373,-1.5918940804\H,-4.4777941121,-0.804046803,-1.0901875101\H,-2.3285959733,-1.9938332434,-0.611880507\H,-2.4554427432,2.9801526371,-0.7544520428\C,2.3878134338,-0.7916434709,0.1475541361\C,2.4598584501,-2.18694634

36,0.0646381164\H,1.5555736948,-2.7541704203,-0.1268102934\C,3.6802562
325,-2.8396904905,0.2269878631\H,3.7231855763,-3.9227373345,0.16054448
77\C,4.8414476175,-2.106836471,0.4729464803\C,4.7747203423,-0.71519364
87,0.5561802647\H,5.6735976578,-0.1373325789,0.7492880349\C,3.55640283
65,-0.0597907657,0.3952486952\H,3.5062540739,1.0215587623,0.4638658129
\H,5.7922014251,-2.6160252031,0.5997608746\O,-4.7931688784,1.699129833
8,-1.23853936\C,-4.8916609214,3.1169684205,-1.2865441638\H,-5.93287962
51,3.335889743,-1.5207778353\H,-4.245098212,3.5282744319,-2.0689535828
\H,-4.63177974,3.5601529472,-0.3188666546\H,0.4017882286,7.1417465424,
0.2164195863\Version=ES64L-G16RevC.01\State=2-A\HF=-1010.859985\S2=0.
769864\S2-1=0.\S2A=0.750228\RMSD=2.137e-09\RMSF=2.558e-06\Dipole=-0.96
49264,2.2800262,-0.1864578\Quadrupole=3.350548,8.362873,-11.7134211,-7
.0903239,-0.7940484,-0.0191101\PG=C01 [X(C20H16N3O1)]\@

7-nitro radical

NO2-Ph-Ph.as

1\1\GINC-GADI-CPU-CLX-2428\FOpt\RM062X\6-31+G(d,p)\C19H13N4O2(1-)\FJR5
02\20-Feb-2020\0\#\M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultraf
ine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\NO2-Ph-Ph.as
\-1,1\C,-3.5839112521,1.260579473,-0.674218546\C,-3.6114435207,-0.093
4543489,-0.328727327\C,-2.4443552382,-0.7118479452,0.0769982759\C,-1.2
220981576,0.0011646935,0.1653558952\C,-1.2559184897,1.4146663727,-0.09
28037162\C,-2.3942683628,2.020024687,-0.5712743909\N,-0.0480422279,2.0
778075143,0.2156562825\N,-0.0670839837,-0.635976169,0.4417833547\C,1.0
601019224,0.0936117919,0.1836721201\N,1.1453992923,1.3752343159,-0.017
9934394\C,0.0830418315,3.4736715095,0.249618604\C,-0.890059616,4.25985
89898,0.8940399552\H,-1.7538251385,3.7847348327,1.348040034\C,-0.74080
32886,5.6392568718,0.9702299175\H,-1.5029763645,6.2250264183,1.4762750
413\C,0.3792116256,6.2703999468,0.4205570216\H,0.4913237506,7.34810248
23,0.4847923871\C,1.3519092315,5.4909007876,-0.2017811572\H,2.23310477
7,5.9603782733,-0.6303758287\C,1.213610166,4.1056994439,-0.2913390229\
H,1.9760878658,3.5056134177,-0.7718154234\C,2.3422477038,-0.6708846215
,0.0823171551\C,2.324734243,-2.0686439209,0.023672576\H,1.3705694872,-
2.5828857787,0.0524998261\C,3.5161926105,-2.7883469825,-0.0728736468\H
,3.4863570153,-3.8731111177,-0.1198671111\C,4.7390544713,-2.1204037971
, -0.1105292657\C,4.7639986822,-0.7249075129,-0.0469219266\H,5.71254424
04,-0.1961607976,-0.0686016296\C,3.5762227559,-0.0059756208,0.05117690
83\H,3.5951625911,1.077453697,0.1092055378\H,-4.5412897405,-0.64647682
04,-0.3937660162\H,-2.4330157631,-1.7694161026,0.3209037966\H,-2.41572
75452,3.0732079373,-0.8200301715\H,5.6666925379,-2.6804027933,-0.18511
6399\N,-4.7747065161,1.8958454446,-1.1170716645\O,-5.8137528035,1.2314
769875,-1.2158761748\O,-4.7396787926,3.0989684405,-1.4000318312\Versi
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74e-06\Dipole=3.3268412,0.0762513,0.6081575\Quadrupole=-22.8504093,14.
4723436,8.3780657,7.9525662,-14.3940528,4.6695896\PG=C01 [X(C19H13N4O2
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NO2-Ph-Ph.cs

1\1\GINC-GADI-CPU-CLX-0363\FOpt\RM062X\6-31+G(d,p)\C19H13N4O2(1+)\FJR5
02\21-Feb-2020\0\#\M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultraf
ine) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\NO2-Ph-Ph.cs
\1,1\C,-3.5825282057,1.3563491764,-0.5760435642\C,-3.6260650133,-0.06
0691665,-0.4969548886\C,-2.4660754358,-0.7491836502,-0.2915762049\C,-1
.2391757876,-0.0406926863,-0.1527105492\C,-1.2550587702,1.3868875303,-
0.1843581121\C,-2.4506134599,2.1026044654,-0.4327037319\N,-0.048000592
5,1.9940347975,0.0117091472\N,-0.0900170456,-0.7109631177,-0.022885318
1\C,1.0299661757,-0.0087015757,0.0549622378\N,1.0635887756,1.349141998
7,0.110657785\C,0.082880456,3.4378689301,0.1159398544\C,-0.6529746125,
4.1184848251,1.0819807476\H,-1.3238314775,3.5881218746,1.7504574975\C,
-0.4732497283,5.4947307388,1.1882512851\H,-1.0251552208,6.0468675886,1
.9411785985\C,0.4174029517,6.1542672658,0.3405886502\H,0.5487466079,7.
2278232867,0.429115556\C,1.1462600745,5.443642623,-0.6146982782\H,1.83
85334082,5.9602211812,-1.270620209\C,0.9910922765,4.0657222024,-0.7306
017711\H,1.5478075941,3.4883838137,-1.4617133694\C,2.3333022466,-0.692

5720878,0.1128049054\C,2.3812109546,-2.0870795918,-0.0206459032\H,1.46
30797245,-2.647389718,-0.15990724\C,3.6062200263,-2.743223618,0.021674
5109\H,3.6424196861,-3.8225395327,-0.0846075361\C,4.7848779613,-2.0160
198116,0.1986925759\C,4.7379645336,-0.6277021658,0.3324319354\H,5.6535
005343,-0.0622342961,0.4719048653\C,3.517256381,0.0379039957,0.2892622
129\H,3.4825354564,1.1166297755,0.3952392063\H,-4.5732331644,-0.572722
4299,-0.6172165789\H,-2.440413447,-1.8321770557,-0.2483785853\H,-2.470
4041988,3.1814719262,-0.523348796\H,5.7397759631,-2.5315550779,0.23194
01787\N,-4.8454066976,2.0757504499,-0.8490721518\O,-5.8514866327,1.404
5476642,-0.9763526382\O,-4.8001222977,3.2887819705,-0.9286163241\\Vers
ion=ES64L-G16RevC.01\State=1-A\HF=-1100.6247982\RMSD=6.792e-09\RMSF=1.
594e-05\Dipole=1.3350469,0.0912894,0.3711805\Quadrupole=-5.8090969,19.
8879603,-14.0788634,5.1027283,-5.4537644,4.0088009\PG=C01 [X(C19H13N4O
2)]\@

NO2-Ph-Ph.nd

1\1\GINC-GADI-CPU-CLX-2426\FOpt\UM062X\6-31+G(d,p)\C19H13N4O2(2)\FJR50
2\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafi
ne) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\\NO2-Ph-Ph.nd\
\,2\C,-3.6141760271,1.335779711,-0.5684790247\C,-3.6360553131,-0.0635
476272,-0.5237368057\C,-2.4474231118,-0.734798239,-0.3305574351\C,-1.2
340957947,-0.0306468622,-0.1725625072\C,-1.2637157485,1.3923414426,-0.
1855570838\C,-2.4558704473,2.0821641628,-0.4107133397\N,-0.0446159125,
2.025942286,0.0096715534\N,-0.0689623686,-0.7160337314,-0.0333994084\C
,1.0450622089,0.0187736701,0.0362748996\N,1.1171661516,1.34761022,0.05
88320536\C,0.0882182039,3.4493971827,0.1102782014\C,-0.629650355,4.144
4248179,1.082596561\H,-1.2921633498,3.6109358375,1.7576310827\C,-0.470
2421045,5.524934256,1.1811211607\H,-1.0224401152,6.0737084252,1.937243
1035\C,0.4029564219,6.1946674034,0.3233316139\H,0.525352246,7.26999359
04,0.4063666395\C,1.1232841138,5.4829441381,-0.6369184024\H,1.80462998
99,6.0014635666,-1.3038388989\C,0.9691148663,4.1031557529,-0.74936493\
H,1.5201656386,3.5319893433,-1.4897232838\C,2.3495914899,-0.6958053015
,0.106275688\C,2.3872390103,-2.0865695472,-0.0476564823\H,1.4629565741
, -2.6284179726,-0.2153925462\C,3.6022671785,-2.7655410211,0.01105897\H
,3.6217998394,-3.8440746954,-0.1120988996\C,4.7885261582,-2.0636749004
,0.225334132\C,4.7547865941,-0.6768665856,0.3808867749\H,5.674382388,-
0.12540892,0.5511249957\C,3.5430755447,0.0059652309,0.3217302354\H,3.5
177573592,1.083165398,0.4462026175\H,-4.5705799747,-0.5967390733,-0.64
81282519\H,-2.4131073564,-1.8186377224,-0.3064342955\H,-2.4901769883,3
.1624053145,-0.46769521\H,5.7349740836,-2.5940760914,0.2717863882\N,-4
.8651219852,2.0501587855,-0.7991170256\O,-5.8843617836,1.391509834,-0.
9483026827\O,-4.8359373246,3.2721979216,-0.8322901575\\Version=ES64L-G
16RevC.01\State=2-A\HF=-1100.8112599\S2=0.769173\S2-1=0.\S2A=0.750253\
RMSD=4.299e-09\RMSF=7.342e-06\Dipole=1.9595716,0.4654407,0.3767839\Qua
drupole=-15.8456658,16.7278491,-0.8821833,7.8034055,-7.0853972,3.57148
45\PG=C01 [X(C19H13N4O2)]\@

Blatter's radical

Ph-Ph-Ph.as

1\1\GINC-GADI-CPU-CLX-1336\FOpt\RM062X\6-31+G(d,p)\C19H14N3(1-)\FJR502
\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafin
e) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\\Ph-Ph-Ph.as\\-
1,1\C,-3.6209998134,1.2587601388,-0.8595716251\C,-3.6306186019,-0.0677
639382,-0.4341914651\C,-2.4568903456,-0.6630559681,0.0359803872\C,-1.2
608780048,0.0636813918,0.1265470627\C,-1.289528748,1.4353321791,-0.232
2843768\C,-2.4383237866,2.0062036552,-0.7737432954\N,-0.0698698037,2.1
113950958,-0.0091095078\N,-0.0736104115,-0.5498608828,0.4899203622\C,1
.0215344104,0.1238693421,0.096124963\N,1.1106745127,1.3779273795,-0.29
44803106\C,0.080125155,3.4742993006,0.1588740932\C,-0.9555832447,4.269
2862023,0.7031979874\H,-1.8945670695,3.8102132897,0.9907545241\C,-0.77
04148447,5.6305222378,0.9075790723\H,-1.5838951823,6.2096484793,1.3368
559381\C,0.4392560353,6.2553375642,0.5864848523\H,0.5744198451,7.32003
56072,0.7478027143\C,1.4693976817,5.4728632116,0.06618861\H,2.42369534
86,5.9292401615,-0.1844924842\C,1.3059044253,4.1053063132,-0.145883728

\H,2.1173843396,3.5107852588,-0.5444702552\C,2.3075850455,-0.648363690
6,0.0363891355\C,2.2942632335,-2.0468784939,0.077633784\H,1.3391456627
, -2.5563366954,0.1472286905\C,3.4859316408,-2.7702147855,0.0276299249
H,3.4587316335,-3.8557652081,0.0594572629\C,4.7079666151,-2.1043163342
, -0.0663293838\H,5.6362779666,-2.6670114906,-0.1056029073\C,4.72999850
65,-0.708582568,-0.1053148303\H,5.6773304905,-0.1810919599,-0.17191479
32\C,3.5397258583,0.0132783686,-0.0504796544\H,3.5543126145,1.09820571
76,-0.0685453515\H,-4.5224488309,1.7223834978,-1.2485835828\H,-4.54707
58495,-0.6496495809,-0.4817930746\H,-2.4435214465,-1.7083187078,0.3343
290003\H,-2.4274450378,3.0418359114,-1.0983777388\\Version=ES64L-G16Re
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.6089822,0.7411932,-0.2061661\Quadrupole=6.0316418,-2.0481718,-3.98347
, -2.3674674,-0.6504395,1.316787\PG=C01 [X(C19H14N3)]\@

Ph-Ph-Ph.cs

1\1\GINC-GADI-CPU-CLX-2904\FOpt\RM062X\6-31+G(d,p)\C19H14N3(1+)\FJR502
\20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine)
OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\Ph-Ph-Ph.cs\1
,1\C,-3.6151547649,1.447231934,-0.6521614658\C,-3.6309528342,0.0186512
223,-0.6212263765\C,-2.4814920433,-0.6943368259,-0.4361810038\C,-1.252
323891,0.0013985175,-0.2584097174\C,-1.2641401436,1.4355563977,-0.2393
835739\C,-2.4621564999,2.1597088651,-0.4665017207\N,-0.0573955913,2.02
06824761,-0.0136823217\N,-0.1102603741,-0.6755122452,-0.1313146996\C,1
.0133006893,0.0187566911,0.0058241706\N,1.0562067484,1.3652290917,0.09
29125668\C,0.0845736082,3.4607389107,0.1226642555\C,-0.6282985668,4.11
86133624,1.1194724409\H,-1.2912040883,3.5693882783,1.7813177938\C,-0.4
444796286,5.4921235064,1.2562119963\H,-0.9805179374,6.0273536285,2.032
7988776\C,0.4294162901,6.1717653304,0.4067140032\H,0.5643550079,7.2428
937617,0.5181698181\C,1.1361477992,5.4837274706,-0.5806258359\H,1.8162
657807,6.0148783742,-1.2381169571\C,0.9742686975,4.1088474922,-0.72684
71488\H,1.5158284416,3.5487046354,-1.4825950691\C,2.3088220521,-0.6861
961532,0.0973654396\C,2.338368928,-2.0842859271,0.0171388908\H,1.41328
37326,-2.6365134785,-0.1075081199\C,3.5532258407,-2.7575740266,0.09791
74939\H,3.5723748116,-3.8409691602,0.0354934598\C,4.741471532,-2.04317
25807,0.2577004756\H,5.6880578708,-2.5712140286,0.3200483902\C,4.71300
41951,-0.6502276211,0.3373423678\H,5.6356438114,-0.0926129942,0.462085
9857\C,3.502151984,0.0309214848,0.2582326214\H,3.4825382197,1.11356183
78,0.3223881973\H,-4.5426771123,1.9795970696,-0.8339923602\H,-4.574090
4413,-0.4977335358,-0.7650194653\H,-2.4582431529,-1.7785510669,-0.4334
301526\H,-2.457928971,3.2417693051,-0.5009932569\\Version=ES64L-G16Rev
C.01\State=1-A\HF=-896.2027427\RMSD=8.767e-09\RMSF=8.430e-06\Dipole=-2
.5498637,1.2335647,-0.3242502\Quadrupole=14.7689525,9.3578083,-24.1267
608,-3.2528505,0.9681179,2.2740526\PG=C01 [X(C19H14N3)]\@

Ph-Ph-Ph.nd

1\1\GINC-GADI-CPU-CLX-0126\FOpt\UM062X\6-31+G(d,p)\C19H14N3(2)\FJR502\
20-Feb-2020\0\#\ M062X/6-31+G** SCF=XQC IOP(2/17=4) INT(grid=ultrafine)
) OPT SCRF=(SMD,Solvent=dichloromethane) maxdisk=50GB\Ph-Ph-Ph.nd\0,
2\C,-3.6537554759,1.4160717265,-0.6422663431\C,-3.657633776,0.01247291
82,-0.6163462641\C,-2.4757430017,-0.6806799182,-0.4182253333\C,-1.2637
69433,0.0084601827,-0.2280189924\C,-1.2830486472,1.4262075754,-0.21750
44263\C,-2.4773056329,2.125480682,-0.4486285078\N,-0.0603440618,2.0490
511036,0.003488458\N,-0.0942921935,-0.6940568988,-0.082887162\C,1.0163
704053,0.0314098496,0.013407882\N,1.101302086,1.3618038439,0.056934417
7\C,0.0839238209,3.4668838334,0.1276896465\C,-0.6468455953,4.158287076
5,1.0937974316\H,-1.3299235056,3.6213036114,1.7452443393\C,-0.47479285
52,5.5352587757,1.2179065422\H,-1.037850948,6.0785191124,1.9703267779\
C,0.4258205612,6.2090631871,0.3920501585\H,0.5589911027,7.2814578649,0
.4953686141\C,1.1604472865,5.5029123901,-0.5613727466\H,1.8644736289,6
.023095931,-1.2033363756\C,0.9921402778,4.1269977823,-0.699188359\H,1.
5553151981,3.5611957043,-1.4346372484\C,2.3200538882,-0.6911720537,0.0
946422512\C,2.3497436554,-2.0857995882,-0.0201999833\H,1.4206056398,-2
.6256949973,-0.1663103797\C,3.5604672677,-2.7717561454,0.0518048012\H,
3.5712384175,-3.8537850701,-0.039137876\C,4.7533097582,-2.0730746433,0

.2385369863\H,5.6964415937,-2.6085081168,0.294406405\C,4.7285741884,-0.6823656815,0.3538632676\H,5.6527491897,-0.131671778,0.5012088103\C,3.5201741946,0.0064390982,0.2830658584\H,3.5027222121,1.0869265723,0.3761998222\H,-4.5766584548,1.9588417183,-0.8191964333\H,-4.5865483601,-0.5289838307,-0.7637951993\H,-2.4466641693,-1.7660193341,-0.4151782289\H,-2.4816982626,3.2086275161,-0.4799026108\\Version=ES64L-G16RevC.01\State=2-A\HF=-896.3751559\S2=0.768198\S2-1=0.\S2A=0.750195\RMSD=2.302e-09\RMSF=3.521e-06\Dipole=-0.7909845,1.6109365,-0.0716177\Quadrupole=6.3760181,6.0137597,-12.3897777,-2.7058653,-1.261043,1.6902417\PG=C01 [X(C19H14N3)]\@

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