R.
Supporting Information

S. Alkylation of Nitroaromatics with Trialkylborane

Section 19.01 N. Palani, Karamil Jayaprakash and Shmaryahu Hoz*

Archive files containing energies and structures of the DFT computed radical anions of Chart 2 and the corresponding coordinates. Figure S1 ^1H NMR and Figure S2 ^{13}C NMR for compound **2g**.

S1

4-CYANONITROBENZENE RADICAL ANION

1\1\GINC-ESHEL\FOpt\UB3LYP\6-31G(d)\C7H4N2O2(1-,2)\ROZENTE\02-Jan-2003 1\1\#P
 B3LYP/6-31G* OPT=Z-MATRIX NOSYMM\4-Cyanonitrobenzene radical anion\1-
 1,2\CC,1,R2\CC,2,R3,1,A3\CC,3,R4,2,A4,1,D4,0\CC,4,R5,3,A5,2,D5,0\CC,1,R6,2,A6,3,
 D6,0\N,1,R7,2,A7,3,D7,0\H,2,R8,1,A8,6,D8,0\H,3,R9,2,A9,1,D9,0\CC,4,R10,3,A10,2,D10,0
 \H,5,R11,4,A11,3,D11,0\H,6,R12,1,A12,2,D12,0\O,7,R13,1,A13,6,D13,0\O,7,R14,1,A14,6,
 D14,0\X,10,1,4,90,3,180,0\N,10,R16,15,A16,4,D16,0\R2=1.42214632\R3=1.37636445\
 R4=1.42598395\R5=1.42611824\R6=1.42218807\R7=1.39644374\R8=1.08293361\R9=
 1.08742282\R10=1.4149867\R11=1.08742966\R12=1.08291779\R13=1.27365969\R14=
 1.27367381\R16=1.1726347\A3=120.29155593\A4=121.21199237\A5=117.913149\A6=
 119.08200407\A7=120.4354978\A8=117.97112279\A9=119.9262878\A10=121.06582157
 \A11=118.85073262\A12=117.97102521\A13=118.83269218\A14=118.86829063\A16
 =89.97191472\A4=0.00121877\A5=0.00045829\A6=0.00215373\A7=-180.00039262\A8=-
 179.99771824\A9=179.99906537\A10=-179.99976789\A11=180.00181514\A12=
 179.99808882\A13=-180.00191025\A14=-0.00953652\A16=180.00000432\Version=IBM-RS6000-
 G98RevA.7\HF=-529.0421047\S2=0.758296\S2-1=0.\S2A=0.75004\RMSD= 3.932e-
 09\RMSF=6.474e-05\Dipole=0.5000194,-0.0000907,0.2941607\PG=C01 [X(C7H4N2O2)]\@

4-CHO-NITROBENZENE RADICAL ANION

1\1\GINC-ARMON\FOpt\UB3LYP\6-31G(d)\C7H5N1O3(1-,2)\ROZENTE\02-Jan-2003 1\1\#P
 B3LYP/6-31G* OPT=Z-MATRIX NOSYMM\4-CHO-Nitrobenzene radical anion\1-
 1,2\CC,1,R2\CC,2,R3,1,A3\CC,3,R4,2,A4,1,D4,0\CC,4,R5,3,A5,2,D5,0\CC,1,R6,2,
 A6,3,D6,0\N,1,R7,2,A7,3,D7,0\H,2,R8,1,A8,6,D8,0\H,3,R9,2,A9,1,D9,0\CC,4,R10,3,A10,
 2,D10,0\H,5,R11,4,A11,3,D11,0\H,6,R12,1,A12,2,D12,0\O,7,R13,1,A13,6,D13,0\O,7,
 R14,1,A14,6,D14,0\O,10,R15,4,A15,3,D15,0\H,10,R16,15,A16,4,D16,0\R2=1.42048374
 \R3=1.37680331\R4=1.42268393\R5=1.42570015\R6=1.42186463\R7=1.40257985\R8=
 1.08319399\R9=1.0903666\R10=1.44043858\R11=1.08687207\R12=1.08353502\R13=
 1.26892193\R14=1.26858612\R15=1.24052737\R16=1.11911455\A3=119.76039995\A4=
 121.84159113\A5=117.47673333\A6=119.34181274\A7=120.26556053\A8=118.12228532
 \A9=119.58257545\A10=120.93636646\A11=117.71481917\A12=117.92549774\A13=118.
 87832955\A14=118.98658344\A15=126.87413144\A16=119.3818732\A4=0.00004974\A5=-
 0.00001048\A6=-0.00005418\A7=-179.99990878\A8=-180.00005387\A9=180.00000416\A10=-
 180.00006554\A11=179.99992005\A12=180.00004729\A13=-179.99972209\A14= 0.00038279\A15=-
 179.99995852\A16=180.00000473\Version=IBM-RS6000-G98RevA.7\HF=-
 550.1247794\S2=0.758873\S2-1=0.\S2A=0.750027\RMSD=8.043e-09\RMSF=1.766e -
 05\Dipole=0.4067665,-0.0000013,0.8858639\PG=C01 [X(C7H5N1O3)]\@

4-CH3SO2-NITROBENZENE RADICAL ANION

1\1\GINC-ARMON\FOpt\UB3LYP\6-31G(d)\C7H7N1O4S1(1-,2)\ROZENTE\03-Feb-20 03\1\#P
 B3LYP/6-31G* OPT=Z-MATRIX NOSYMM\4-CH3SO2-Nitrobenzene radical anion\1-
 1,2\CC,1,R2\CC,2,R3,1,A3\CC,3,R4,2,A4,1,D4,0\CC,4,R5,3,A5,2,D5,0\CC,1,
 R6,2,A6,3,D6,0\N,1,R7,2,A7,3,D7,0\H,2,R8,1,A8,6,D8,0\H,3,R9,2,A9,1,D9,0\S,4,R10,3,
 A10,2,D10,0\H,5,R11,4,A11,3,D11,0\H,6,R12,1,A12,2,D12,0\O,7,R13,1,A13,6,D13,0\O,
 7,R14,1,A14,6,D14,0\O,10,R15,4,A15,3,D15,0\O,10,R16,4,A16,3,D16,0\CC,10,R17,15,A
 17,4,D17,0\H,17,R18,10,A18,4,D18,0\H,17,R19,10,A19,4,D19,0\H,17,R20,10,A20,4,D20
 ,0\R2=1.42315833\R3=1.37778464\R4=1.41843335\R5=1.41838111\R6=1.42312655\R7
 =1.39613886\R8=1.08283056\R9=1.0861575\R10=1.74934965\R11=1.08617411\R12=
 1.08283067\R13=1.27427391\R14=1.27428317\R15=1.48026855\R16=1.48026055\R17=
 1.82350296\R18=1.0921377\R19=1.09212423\R20=1.09382926\A3=120.24766791\A4=
 120.3100173\A5=119.57319577\A6=119.30181465\A7=120.33131221\A8=117.9868408
 5\A9=120.49873768\A10=120.08554889\A11=119.18332798\A12=117.98753919\A13=
 118.80200473\A14=118.824044\A15=109.87314169\A16=109.89001669\A17=105.2951
 0812\A18=108.93978677\A19=108.93584839\A20=107.40348268\A4=0.47842154\A5=-
 0.1767155\A6=-0.81409383\A7=-180.70981897\A8=-181.22157199\A9=179.13091497\A10=-

174.23787423\N11=178.85462272\N12=181.20300571\N13=-180.0060384\N14=0.08267649\N15=-
 159.87772092\N16=-26.04586941\N17=113.28858956\N18=-60.19014155\N19=60.53494875\N20=-
 179.82822684\Version=IBM-RS6000-G98RevA.7\HF=-1024.6837421\N2=0.755899\N2-
 1=0\N2A=0.75002\N2RMSD=6.693e-09\N2RMSF=3.056e-05\N2Dipole=2.1671521,-
 1.3531307,1.2570497\PG=C01 [X(C7H7N1O4S1)]\@

1,4-DINITRO-6-ME-BENZENE RADICAL ANION

1\GINC-ARMONFOpt\UB3LYP\6-31G(d)\C7H6N2O4(1,2)\ROZENITE\19-Jan-2003\1\#P
 B3LYP/6-31G* OPT=Z-MATRIX NOSYMM\1,4-Dinitro-6-Me-benzene radical anion\ -
 1,2\N1C,1,R2\N2C,2,R3,1,A3\N3C,3,R4,2,A4,1,D4,0\N4C,4,R5,3,A5,2,D5,0\N5C,5,R6,2,A6,3
 ,D6,0\N6C,6,R7,2,A7,3,D7,0\N7C,7,R8,1,A8,6,D8,0\N8C,8,R9,2,A9,1,D9,0\N9C,9,R10,3,A10,2,D10,
 0\N10C,10,R11,4,A11,3,D11,0\N11C,11,R12,1,A12,2,D12,0\N12C,12,R13,1,A13,6,D13,0\N13C,13,R14,1,A14,
 6,D14,0\N14C,14,R15,4,A15,3,D15,0\N15C,15,R16,15,A16,4,D16,0\N16C,16,R17,6,A17,1,D17,0\N17C,17,R18,6,
 A18,1,D18,0\N18C,18,R19,6,A19,1,D19,0\N19C,19,R20,6,A20,1,D20,0\N20C,20,R21,6,A21,1,D21,0\N21C,21,
 R22,6,A22,1,D22,0\N22C,22,R23,6,A23,1,D23,0\N23C,23,R24,6,A24,1,D24,0\N24C,24,R25,6,A25,1,D25,0\N25C,25,
 R26,6,A26,1,D26,0\N26C,26,R27,6,A27,1,D27,0\N27C,27,R28,6,A28,1,D28,0\N28C,28,R29,6,A29,1,D29,0\N29C,29,
 R30,6,A30,1,D30,0\N30C,30,R31,6,A31,1,D31,0\N31C,31,R32,6,A32,1,D32,0\N32C,32,R33,6,A33,1,D33,0\N33C,33,
 R34,6,A34,1,D34,0\N34C,34,R35,6,A35,1,D35,0\N35C,35,R36,6,A36,1,D36,0\N36C,36,R37,6,A37,1,D37,0\N37C,37,
 R38,6,A38,1,D38,0\N38C,38,R39,6,A39,1,D39,0\N39C,39,R40,6,A40,1,D40,0\N40C,40,R41,6,A41,1,D41,0\N41C,41,
 R42,6,A42,1,D42,0\N42C,42,R43,6,A43,1,D43,0\N43C,43,R44,6,A44,1,D44,0\N44C,44,R45,6,A45,1,D45,0\N45C,45,
 R46,6,A46,1,D46,0\N46C,46,R47,6,A47,1,D47,0\N47C,47,R48,6,A48,1,D48,0\N48C,48,R49,6,A49,1,D49,0\N49C,49,
 R50,6,A50,1,D50,0\N50C,50,R51,6,A51,1,D51,0\N51C,51,R52,6,A52,1,D52,0\N52C,52,R53,6,A53,1,D53,0\N53C,53,
 R54,6,A54,1,D54,0\N54C,54,R55,6,A55,1,D55,0\N55C,55,R56,6,A56,1,D56,0\N56C,56,R57,6,A57,1,D57,0\N57C,57,
 R58,6,A58,1,D58,0\N58C,58,R59,6,A59,1,D59,0\N59C,59,R60,6,A60,1,D60,0\N60C,60,R61,6,A61,1,D61,0\N61C,61,
 R62,6,A62,1,D62,0\N62C,62,R63,6,A63,1,D63,0\N63C,63,R64,6,A64,1,D64,0\N64C,64,R65,6,A65,1,D65,0\N65C,65,
 R66,6,A66,1,D66,0\N66C,66,R67,6,A67,1,D67,0\N67C,67,R68,6,A68,1,D68,0\N68C,68,R69,6,A69,1,D69,0\N69C,69,
 R70,6,A70,1,D70,0\N70C,70,R71,6,A71,1,D71,0\N71C,71,R72,6,A72,1,D72,0\N72C,72,R73,6,A73,1,D73,0\N73C,73,
 R74,6,A74,1,D74,0\N74C,74,R75,6,A75,1,D75,0\N75C,75,R76,6,A76,1,D76,0\N76C,76,R77,6,A77,1,D77,0\N77C,77,
 R78,6,A78,1,D78,0\N78C,78,R79,6,A79,1,D79,0\N79C,79,R80,6,A80,1,D80,0\N80C,80,R81,6,A81,1,D81,0\N81C,81,
 R82,6,A82,1,D82,0\N82C,82,R83,6,A83,1,D83,0\N83C,83,R84,6,A84,1,D84,0\N84C,84,R85,6,A85,1,D85,0\N85C,85,
 R86,6,A86,1,D86,0\N86C,86,R87,6,A87,1,D87,0\N87C,87,R88,6,A88,1,D88,0\N88C,88,R89,6,A89,1,D89,0\N89C,89,
 R90,6,A90,1,D90,0\N90C,90,R91,6,A91,1,D91,0\N91C,91,R92,6,A92,1,D92,0\N92C,92,R93,6,A93,1,D93,0\N93C,93,
 R94,6,A94,1,D94,0\N94C,94,R95,6,A95,1,D95,0\N95C,95,R96,6,A96,1,D96,0\N96C,96,R97,6,A97,1,D97,0\N97C,97,
 R98,6,A98,1,D98,0\N98C,98,R99,6,A99,1,D99,0\N99C,99,R100,6,A100,1,D100,0\N100C,100,R101,6,A101,1,D101,0\N101C,101,
 R102,6,A102,1,D102,0\N102C,102,R103,6,A103,1,D103,0\N103C,103,R104,6,A104,1,D104,0\N104C,104,R105,6,A105,1,D105,0\N105C,105,
 R106,6,A106,1,D106,0\N106C,106,R107,6,A107,1,D107,0\N107C,107,R108,6,A108,1,D108,0\N108C,108,R109,6,A109,1,D109,0\N109C,109,
 R110,6,A110,1,D110,0\N110C,110,R111,6,A111,1,D111,0\N111C,111,R112,6,A112,1,D112,0\N112C,112,R113,6,A113,1,D113,0\N113C,113,
 R114,6,A114,1,D114,0\N114C,114,R115,6,A115,1,D115,0\N115C,115,R116,6,A116,1,D116,0\N116C,116,R117,6,A117,1,D117,0\N117C,117,
 R118,6,A118,1,D118,0\N118C,118,R119,6,A119,1,D119,0\N119C,119,R120,6,A120,1,D120,0\N120C,120,R121,6,A121,1,D121,0\N121C,121,
 R122,6,A122,1,D122,0\N122C,122,R123,6,A123,1,D123,0\N123C,123,R124,6,A124,1,D124,0\N124C,124,R125,6,A125,1,D125,0\N125C,125,
 R126,6,A126,1,D126,0\N126C,126,R127,6,A127,1,D127,0\N127C,127,R128,6,A128,1,D128,0\N128C,128,R129,6,A129,1,D129,0\N129C,129,
 R130,6,A130,1,D130,0\N130C,130,R131,6,A131,1,D131,0\N131C,131,R132,6,A132,1,D132,0\N132C,132,R133,6,A133,1,D133,0\N133C,133,
 R134,6,A134,1,D134,0\N134C,134,R135,6,A135,1,D135,0\N135C,135,R136,6,A136,1,D136,0\N136C,136,R137,6,A137,1,D137,0\N137C,137,
 R138,6,A138,1,D138,0\N138C,138,R139,6,A139,1,D139,0\N139C,139,R140,6,A140,1,D140,0\N140C,140,R141,6,A141,1,D141,0\N141C,141,
 R142,6,A142,1,D142,0\N142C,142,R143,6,A143,1,D143,0\N143C,143,R144,6,A144,1,D144,0\N144C,144,R145,6,A145,1,D145,0\N145C,145,
 R146,6,A146,1,D146,0\N146C,146,R147,6,A147,1,D147,0\N147C,147,R148,6,A148,1,D148,0\N148C,148,R149,6,A149,1,D149,0\N149C,149,
 R150,6,A150,1,D150,0\N150C,150,R151,6,A151,1,D151,0\N151C,151,R152,6,A152,1,D152,0\N152C,152,R153,6,A153,1,D153,0\N153C,153,
 R154,6,A154,1,D154,0\N154C,154,R155,6,A155,1,D155,0\N155C,155,R156,6,A156,1,D156,0\N156C,156,R157,6,A157,1,D157,0\N157C,157,
 R158,6,A158,1,D158,0\N158C,158,R159,6,A159,1,D159,0\N159C,159,R160,6,A160,1,D160,0\N160C,160,R161,6,A161,1,D161,0\N161C,161,
 R162,6,A162,1,D162,0\N162C,162,R163,6,A163,1,D163,0\N163C,163,R164,6,A164,1,D164,0\N164C,164,R165,6,A165,1,D165,0\N165C,165,
 R166,6,A166,1,D166,0\N166C,166,R167,6,A167,1,D167,0\N167C,167,R168,6,A168,1,D168,0\N168C,168,R169,6,A169,1,D169,0\N169C,169,
 R170,6,A170,1,D170,0\N170C,170,R171,6,A171,1,D171,0\N171C,171,R172,6,A172,1,D172,0\N172C,172,R173,6,A173,1,D173,0\N173C,173,
 R174,6,A174,1,D174,0\N174C,174,R175,6,A175,1,D175,0\N175C,175,R176,6,A176,1,D176,0\N176C,176,R177,6,A177,1,D177,0\N177C,177,
 R178,6,A178,1,D178,0\N178C,178,R179,6,A179,1,D179,0\N179C,179,R180,6,A180,1,D180,0\N180C,180,R181,6,A181,1,D181,0\N181C,181,
 R182,6,A182,1,D182,0\N182C,182,R183,6,A183,1,D183,0\N183C,183,R184,6,A184,1,D184,0\N184C,184,R185,6,A185,1,D185,0\N185C,185,
 R186,6,A186,1,D186,0\N186C,186,R187,6,A187,1,D187,0\N187C,187,R188,6,A188,1,D188,0\N188C,188,R189,6,A189,1,D189,0\N189C,189,
 R190,6,A190,1,D190,0\N190C,190,R191,6,A191,1,D191,0\N191C,191,R192,6,A192,1,D192,0\N192C,192,R193,6,A193,1,D193,0\N193C,193,
 R194,6,A194,1,D194,0\N194C,194,R195,6,A195,1,D195,0\N195C,195,R196,6,A196,1,D196,0\N196C,196,R197,6,A197,1,D197,0\N197C,197,
 R198,6,A198,1,D198,0\N198C,198,R199,6,A199,1,D199,0\N199C,199,R200,6,A200,1,D200,0\N200C,200,R201,6,A201,1,D201,0\N201C,201,
 R202,6,A202,1,D202,0\N202C,202,R203,6,A203,1,D203,0\N203C,203,R204,6,A204,1,D204,0\N204C,204,R205,6,A205,1,D205,0\N205C,205,
 R206,6,A206,1,D206,0\N206C,206,R207,6,A207,1,D207,0\N207C,207,R208,6,A208,1,D208,0\N208C,208,R209,6,A209,1,D209,0\N209C,209,
 R210,6,A210,1,D210,0\N210C,210,R211,6,A211,1,D211,0\N211C,211,R212,6,A212,1,D212,0\N212C,212,R213,6,A213,1,D213,0\N213C,213,
 R214,6,A214,1,D214,0\N214C,214,R215,6,A215,1,D215,0\N215C,215,R216,6,A216,1,D216,0\N216C,216,R217,6,A217,1,D217,0\N217C,217,
 R218,6,A218,1,D218,0\N218C,218,R219,6,A219,1,D219,0\N219C,219,R220,6,A220,1,D220,0\N220C,220,R221,6,A221,1,D221,0\N221C,221,
 R222,6,A222,1,D222,0\N222C,222,R223,6,A223,1,D223,0\N223C,223,R224,6,A224,1,D224,0\N224C,224,R225,6,A225,1,D225,0\N225C,225,
 R226,6,A226,1,D226,0\N226C,226,R227,6,A227,1,D227,0\N227C,227,R228,6,A228,1,D228,0\N228C,228,R229,6,A229,1,D229,0\N229C,229,
 R230,6,A230,1,D230,0\N230C,230,R231,6,A231,1,D231,0\N231C,231,R232,6,A232,1,D232,0\N232C,232,R233,6,A233,1,D233,0\N233C,233,
 R234,6,A234,1,D234,0\N234C,234,R235,6,A235,1,D235,0\N235C,235,R236,6,A236,1,D236,0\N236C,236,R237,6,A237,1,D237,0\N237C,237,
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 R

H	-.955316	.000000	1.931053
H	1.191831	.000000	-3.194255
C	3.685706	.000002	2.161936
H	3.377704	.000004	-.519120
H	1.212675	.000002	-1.779944
O	-2.300723	.000006	-.056103
O	-1.183091	-.000003	-1.975182
O	4.832133	.000004	1.688002
H	3.550839	.000002	3.272895

4-CH3SO2-NITROBENZENE RADICAL ANION

HF=-1024.6837421

C	.000000	.000000	.000000
C	.000000	.000000	1.423158
C	1.190208	.000000	2.117202
C	2.425430	.010225	1.420012
C	2.428668	.016665	.001649
C	1.240918	.017633	-.696492
N	-1.204942	-.014928	-.705049
H	-.956175	.006800	1.931297
H	1.195021	.014195	3.203256
S	3.930032	-.141766	2.299384
H	3.377860	.043440	-.525694
H	1.215902	.037355	-1.778854
O	-2.298621	-.030650	-.051295
O	-1.171432	-.014071	-1.978891
O	5.048667	.367483	1.474449
O	3.755316	.348939	3.684972
O	4.226467	-1.933996	2.458131
H	3.396075	-2.383392	3.006998
H	4.307687	-2.369567	1.459924
H	5.162759	-2.063239	3.008692

1,4-DINITRO-6-ME-BENZENE RADICAL ANION

HF=-680.6270889

C	.000000	.000000	.000000
C	.000000	.000000	1.421060
C	1.170251	.000000	2.141316
C	2.405373	.000021	1.455045
C	2.411996	.000041	.041796
C	1.247341	.000033	-.708085
N	-1.260055	.000018	-.644263
H	-.962609	.000000	1.915705
H	1.172892	-.000012	3.224237
N	3.620949	.000029	2.171134
H	3.375877	.000069	-.453185
C	1.374187	.000049	-2.215322
O	-2.304096	.000091	.064542
O	-1.321740	-.000048	-1.905128
O	4.707447	.000034	1.529069
O	3.581715	.000001	3.432715
H	2.435315	.000021	-2.491717
H	.889161	.871827	-2.663895
H	.889099	-.871679	-2.663919

Figure S1

^1H NMR: (300 MHz, CDCl_3 , TMS, δ ppm) 0.877 (d, 3H, 7.5Hz), 1.17 (s, 3H), 1.12-1.15 (m, 1H), 1.30 (s, 3H), 1.84-1.95 (m, 2H), 2.04-2.09 (m, 2H), 2.40-2.57 (2H), 3.09-3.15 (m, 1H), 7.46 (d, 2H, 9Hz), 8.18 (d, 2H, 9Hz)

Figure S2.

^{13}C NMR (75 MHz, CDCl_3 , TMS, δ ppm): 20.9, 23.0, 28.4, 35.0, 37.2, 39.2, 41.7, 45.0, 45.8, 47.9, 123.7, 129.1, 146.2, 157.3.