

Electronic Supplementary Information

An *ab initio* and DFT study of some halogen atom transfer reactions from alkyl group to acyl radical

Hiroshi Matsubara^{*a}, Ilhyong Ryu^a and Carl H. Schiesser^{b,c}

^a Department of Chemistry, Graduate School of Science, Osaka Prefecture University, Sakai, Osaka 599-8531, Japan

^b School of Chemistry, The University of Melbourne, Victoria 3010, Australia

^c Bio21 Molecular Science and Biotechnology Institute, The University of Melbourne, Victoria 3010, Australia

HF/6-311G^{**}, HF/DZP, MP2/6-311G^{**}, MP2/DZP, MP2/cc-pVDZ, BHandHLYP/6-311G^{**}, BHandHLYP/DZP, BHandHLYP/cc-pVDZ, B3LYP/6-311G^{**}, B3LYP/DZP and B3LYP/cc-pVDZ Gaussian Archive entries for the optimized structures in this study and higher-level calculated single-point energies (17 pages).

Transition state for chlorine transfer reaction from methyl chloride 3 (X = Cl, R = CH₃)

UHF/6-311G**

1\1\GINC-G98\PTS\UHF\6-311G(d,p)\C3H6Cl1O1(2)\MATSU\06-Aug-2005\1\#UHF/6-311G** SCF=(DIRECT, NOVARACC) GEOM=CHECK GUESS=READ OPT=(TS,READFC,EF,Z-MATRIX,MAXCYCLES=100) NOSYMM\acetyl radical with CH₃Cl\0,2\Cl\C,1,r1\X,1,1.,2,90.\C,1,r3,3,a2,2,d1,0\O,2,r4,1,a3,3,d2,0\C,2,r5,1,a4,3,d3,0\H,4,r6,1,a5,3,d4,0\H,4,r7,1,a6,3,d5,0\H,4,r8,1,a7,3,d6,0\H,6,r9,2,a8,5,d7,0\H,6,r10,2,a9,5,d8,0\H,6,r11,2,a10,5,d9,0\H,6,r12,2,a11,5,d10,0\H,6,r13,2,a12,5,d11,0\H,6,r14,2,a13,5,d12,0\H,6,r15,2,a14,5,d13,0\H,6,r16,2,a15,5,d14,0\H,6,r17,2,a16,5,d15,0\H,6,r18,2,a17,5,d16,0\H,6,r19,2,a18,5,d17,0\H,6,r20,2,a19,5,d18,0\H,6,r21,2,a20,5,d19,0\H,6,r22,2,a21,5,d20,0\H,6,r23,2,a22,5,d21,0\H,6,r24,2,a23,5,d22,0\H,6,r25,2,a24,5,d23,0\H,6,r26,2,a25,5,d24,0\H,6,r27,2,a26,5,d25,0\H,6,r28,2,a27,5,d26,0\H,6,r29,2,a28,5,d27,0\H,6,r30,2,a29,5,d28,0\H,6,r31,2,a30,5,d29,0\H,6,r32,2,a31,5,d30,0\H,6,r33,2,a32,5,d31,0\H,6,r34,2,a33,5,d32,0\H,6,r35,2,a34,5,d33,0\H,6,r36,2,a35,5,d34,0\H,6,r37,2,a36,5,d35,0\H,6,r38,2,a37,5,d36,0\H,6,r39,2,a38,5,d37,0\H,6,r40,2,a39,5,d38,0\H,6,r41,2,a40,5,d39,0\H,6,r42,2,a41,5,d40,0\H,6,r43,2,a42,5,d41,0\H,6,r44,2,a43,5,d42,0\H,6,r45,2,a44,5,d43,0\H,6,r46,2,a45,5,d44,0\H,6,r47,2,a46,5,d45,0\H,6,r48,2,a47,5,d46,0\H,6,r49,2,a48,5,d47,0\H,6,r50,2,a49,5,d48,0\H,6,r51,2,a50,5,d49,0\H,6,r52,2,a51,5,d50,0\H,6,r53,2,a52,5,d51,0\H,6,r54,2,a53,5,d52,0\H,6,r55,2,a54,5,d53,0\H,6,r56,2,a55,5,d54,0\H,6,r57,2,a56,5,d55,0\H,6,r58,2,a57,5,d56,0\H,6,r59,2,a58,5,d57,0\H,6,r60,2,a59,5,d58,0\H,6,r61,2,a60,5,d59,0\H,6,r62,2,a61,5,d60,0\H,6,r63,2,a62,5,d61,0\H,6,r64,2,a63,5,d62,0\H,6,r65,2,a64,5,d63,0\H,6,r66,2,a65,5,d64,0\H,6,r67,2,a66,5,d65,0\H,6,r68,2,a67,5,d66,0\H,6,r69,2,a68,5,d67,0\H,6,r70,2,a69,5,d68,0\H,6,r71,2,a70,5,d69,0\H,6,r72,2,a71,5,d70,0\H,6,r73,2,a72,5,d71,0\H,6,r74,2,a73,5,d72,0\H,6,r75,2,a74,5,d73,0\H,6,r76,2,a75,5,d74,0\H,6,r77,2,a76,5,d75,0\H,6,r78,2,a77,5,d76,0\H,6,r79,2,a78,5,d77,0\H,6,r80,2,a79,5,d78,0\H,6,r81,2,a80,5,d79,0\H,6,r82,2,a81,5,d80,0\H,6,r83,2,a82,5,d81,0\H,6,r84,2,a83,5,d82,0\H,6,r85,2,a84,5,d83,0\H,6,r86,2,a85,5,d84,0\H,6,r87,2,a86,5,d85,0\H,6,r88,2,a87,5,d86,0\H,6,r89,2,a88,5,d87,0\H,6,r90,2,a89,5,d88,0\H,6,r91,2,a90,5,d89,0\H,6,r92,2,a91,5,d90,0\H,6,r93,2,a92,5,d91,0\H,6,r94,2,a93,5,d92,0\H,6,r95,2,a94,5,d93,0\H,6,r96,2,a95,5,d94,0\H,6,r97,2,a96,5,d95,0\H,6,r98,2,a97,5,d96,0\H,6,r99,2,a98,5,d97,0\H,6,r100,2,a99,5,d98,0\H,6,r101,2,a100,5,d99,0\H,6,r102,2,a101,5,d100,0\H,6,r103,2,a102,5,d101,0\H,6,r104,2,a103,5,d102,0\H,6,r105,2,a104,5,d103,0\H,6,r106,2,a105,5,d104,0\H,6,r107,2,a106,5,d105,0\H,6,r108,2,a107,5,d106,0\H,6,r109,2,a108,5,d107,0\H,6,r110,2,a109,5,d108,0\H,6,r111,2,a110,5,d109,0\H,6,r112,2,a111,5,d110,0\H,6,r113,2,a112,5,d111,0\H,6,r114,2,a113,5,d112,0\H,6,r115,2,a114,5,d113,0\H,6,r116,2,a115,5,d114,0\H,6,r117,2,a116,5,d115,0\H,6,r118,2,a117,5,d116,0\H,6,r119,2,a118,5,d117,0\H,6,r120,2,a119,5,d118,0\H,6,r121,2,a120,5,d119,0\H,6,r122,2,a121,5,d120,0\H,6,r123,2,a122,5,d121,0\H,6,r124,2,a123,5,d122,0\H,6,r125,2,a124,5,d123,0\H,6,r126,2,a125,5,d124,0\H,6,r127,2,a126,5,d125,0\H,6,r128,2,a127,5,d126,0\H,6,r129,2,a128,5,d127,0\H,6,r130,2,a129,5,d128,0\H,6,r131,2,a130,5,d129,0\H,6,r132,2,a131,5,d130,0\H,6,r133,2,a132,5,d131,0\H,6,r134,2,a133,5,d132,0\H,6,r135,2,a134,5,d133,0\H,6,r136,2,a135,5,d134,0\H,6,r137,2,a136,5,d135,0\H,6,r138,2,a137,5,d136,0\H,6,r139,2,a138,5,d137,0\H,6,r140,2,a139,5,d138,0\H,6,r141,2,a140,5,d139,0\H,6,r142,2,a141,5,d140,0\H,6,r143,2,a142,5,d141,0\H,6,r144,2,a143,5,d142,0\H,6,r145,2,a144,5,d143,0\H,6,r146,2,a145,5,d144,0\H,6,r147,2,a146,5,d145,0\H,6,r148,2,a147,5,d146,0\H,6,r149,2,a148,5,d147,0\H,6,r150,2,a149,5,d148,0\H,6,r151,2,a150,5,d149,0\H,6,r152,2,a151,5,d150,0\H,6,r153,2,a152,5,d151,0\H,6,r154,2,a153,5,d152,0\H,6,r155,2,a154,5,d153,0\H,6,r156,2,a155,5,d154,0\H,6,r157,2,a156,5,d155,0\H,6,r158,2,a157,5,d156,0\H,6,r159,2,a158,5,d157,0\H,6,r160,2,a159,5,d158,0\H,6,r161,2,a160,5,d159,0\H,6,r162,2,a161,5,d160,0\H,6,r163,2,a162,5,d161,0\H,6,r164,2,a163,5,d162,0\H,6,r165,2,a164,5,d163,0\H,6,r166,2,a165,5,d164,0\H,6,r167,2,a166,5,d165,0\H,6,r168,2,a167,5,d166,0\H,6,r169,2,a168,5,d167,0\H,6,r170,2,a169,5,d168,0\H,6,r171,2,a170,5,d169,0\H,6,r172,2,a171,5,d170,0\H,6,r173,2,a172,5,d171,0\H,6,r174,2,a173,5,d172,0\H,6,r175,2,a174,5,d173,0\H,6,r176,2,a175,5,d174,0\H,6,r177,2,a176,5,d175,0\H,6,r178,2,a177,5,d176,0\H,6,r179,2,a178,5,d177,0\H,6,r180,2,a179,5,d178,0\H,6,r181,2,a180,5,d179,0\H,6,r182,2,a181,5,d180,0\H,6,r183,2,a182,5,d181,0\H,6,r184,2,a183,5,d182,0\H,6,r185,2,a184,5,d183,0\H,6,r186,2,a185,5,d184,0\H,6,r187,2,a186,5,d185,0\H,6,r188,2,a187,5,d186,0\H,6,r189,2,a188,5,d187,0\H,6,r190,2,a189,5,d188,0\H,6,r191,2,a190,5,d189,0\H,6,r192,2,a191,5,d190,0\H,6,r193,2,a192,5,d191,0\H,6,r194,2,a193,5,d192,0\H,6,r195,2,a194,5,d193,0\H,6,r196,2,a195,5,d194,0\H,6,r197,2,a196,5,d195,0\H,6,r198,2,a197,5,d196,0\H,6,r199,2,a198,5,d197,0\H,6,r200,2,a199,5,d198,0\H,6,r201,2,a200,5,d199,0\H,6,r202,2,a201,5,d200,0\H,6,r203,2,a202,5,d201,0\H,6,r204,2,a203,5,d202,0\H,6,r205,2,a204,5,d203,0\H,6,r206,2,a205,5,d204,0\H,6,r207,2,a206,5,d205,0\H,6,r208,2,a207,5,d206,0\H,6,r209,2,a208,5,d207,0\H,6,r210,2,a209,5,d208,0\H,6,r211,2,a210,5,d209,0\H,6,r212,2,a211,5,d210,0\H,6,r213,2,a212,5,d211,0\H,6,r214,2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BHandHLYP/6-311G**

1\1\GINC-G98\PTS\UBHandHLYP\6-311G(d,p)\C3H6Cl1O1(2)\MATSU\06-Aug-2005\1\#BHANDHLYP/6-311G** SCF=DIRECT GEOM=CHECK GUESS=READ OPT=(TS,READFC,EF,Z-MATRIX,MAXCYCLES=100) NOSYMM\acetyl radical with CH3Cl\0,2\Cl\C,1,r1\X,1,1.,2,90.\C,1,r3,3,a2,2,d1,0\O,2,r4,1,a3,3,d2,0\C,2,r5,1,a4,3,d3,0\H,4,r6,1,a5,3,d4,0\H,4,r7,1,a6,3,d5,0\H,4,r8,1,a7,3,d6,0\H,6,r9,2,a8,5,d7,0\H,6,r10,2,a9,5,d8,0\H,6,r11,2,a10,5,d9,0\H,6,r12,2,a11,5,d10,5,d11,5,d12,5\H,6,r13,2,a12,5,d13,5,d14,5,d15,5,d16,5,d17,5,d18,5,d19,5,d20,5,d21,5,d22,5,d23,5,d24,5,d25,5,d26,5,d27,5,d28,5,d29,5,d30,5,d31,5,d32,5,d33,5,d34,5,d35,5,d36,5,d37,5,d38,5,d39,5,d40,5,d41,5,d42,5,d43,5,d44,5,d45,5,d46,5,d47,5,d48,5,d49,5,d50,5,d51,5,d52,5,d53,5,d54,5,d55,5,d56,5,d57,5,d58,5,d59,5,d60,5,d61,5,d62,5,d63,5,d64,5,d65,5,d66,5,d67,5,d68,5,d69,5,d70,5,d71,5,d72,5,d73,5,d74,5,d75,5,d76,5,d77,5,d78,5,d79,5,d80,5,d81,5,d82,5,d83,5,d84,5,d85,5,d86,5,d87,5,d88,5,d89,5,d90,5,d91,5,d92,5,d93,5,d94,5,d95,5,d96,5,d97,5,d98,5,d99,5,d100,5,d101,5,d102,5,d103,5,d104,5,d105,5,d106,5,d107,5,d108,5,d109,5,d110,5,d111,5,d112,5,d113,5,d114,5,d115,5,d116,5,d117,5,d118,5,d119,5,d120,5,d121,5,d122,5,d123,5,d124,5,d125,5,d126,5,d127,5,d128,5,d129,5,d130,5,d131,5,d132,5,d133,5,d134,5,d135,5,d136,5,d137,5,d138,5,d139,5,d140,5,d141,5,d142,5,d143,5,d144,5,d145,5,d146,5,d147,5,d148,5,d149,5,d150,5,d151,5,d152,5,d153,5,d154,5,d155,5,d156,5,d157,5,d158,5,d159,5,d160,5,d161,5,d162,5,d163,5,d164,5,d165,5,d166,5,d167,5,d168,5,d169,5,d170,5,d171,5,d172,5,d173,5,d174,5,d175,5,d176,5,d177,5,d178,5,d179,5,d180,5,d181,5,d182,5,d183,5,d184,5,d185,5,d186,5,d187,5,d188,5,d189,5,d190,5,d191,5,d192,5,d193,5,d194,5,d195,5,d196,5,d197,5,d198,5,d199,5,d200,5,d201,5,d202,5,d203,5,d204,5,d205,5,d206,5,d207,5,d208,5,d209,5,d210,5,d211,5,d212,5,d213,5,d214,5,d215,5,d216,5,d217,5,d218,5,d219,5,d220,5,d221,5,d222,5,d223,5,d224,5,d225,5,d226,5,d227,5,d228,5,d229,5,d230,5,d231,5,d232,5,d233,5,d234,5,d235,5,d236,5,d237,5,d238,5,d239,5,d240,5,d241,5,d242,5,d243,5,d244,5,d245,5,d246,5,d247,5,d248,5,d249,5,d250,5,d251,5,d252,5,d253,5,d254,5,d255,5,d256,5,d257,5,d258,5,d259,5,d260,5,d261,5,d262,5,d263,5,d264,5,d265,5,d266,5,d267,5,d268,5,d269,5,d270,5,d271,5,d272,5,d273,5,d274,5,d275,5,d276,5,d277,5,d278,5,d279,5,d280,5,d281,5,d282,5,d283,5,d284,5,d285,5,d286,5,d287,5,d288,5,d289,5,d290,5,d291,5,d292,5,d293,5,d294,5,d295,5,d296,5,d297,5,d298,5,d299,5,d300,5,d301,5,d302,5,d303,5,d304,5,d305,5,d306,5,d307,5,d308,5,d309,5,d310,5,d311,5,d312,5,d313,5,d314,5,d315,5,d316,5,d317,5,d318,5,d319,5,d320,5,d321,5,d322,5,d323,5,d324,5,d325,5,d326,5,d327,5,d328,5,d329,5,d330,5,d331,5,d332,5,d333,5,d334,5,d335,5,d336,5,d337,5,d338,5,d339,5,d340,5,d341,5,d342,5,d343,5,d344,5,d345,5,d346,5,d347,5,d348,5,d349,5,d350,5,d351,5,d352,5,d353,5,d354,5,d355,5,d356,5,d357,5,d358,5,d359,5,d360,5,d361,5,d362,5,d363,5,d364,5,d365,5,d366,5,d367,5,d368,5,d369,5,d370,5,d371,5,d372,5,d373,5,d374,5,d375,5,d376,5,d377,5,d378,5,d379,5,d380,5,d381,5,d382,5,d383,5,d384,5,d385,5,d386,5,d387,5,d388,5,d389,5,d390,5,d391,5,d392,5,d393,5,d394,5,d395,5,d396,5,d397,5,d398,5,d399,5,d400,5,d401,5,d402,5,d403,5,d404,5,d405,5,d406,5,d407,5,d408,5,d409,5,d410,5,d411,5,d412,5,d413,5,d414,5,d415,5,d416,5,d417,5,d418,5,d419,5,d420,5,d421,5,d422,5,d423,5,d424,5,d425,5,d426,5,d427,5,d428,5,d429,5,d430,5,d431,5,d432,5,d433,5,d434,5,d435,5,d436,5,d437,5,d438,5,d439,5,d440,5,d441,5,d442,5,d443,5,d444,5,d445,5,d446,5,d447,5,d448,5,d449,5,d450,5,d451,5,d452,5,d453,5,d454,5,d455,5,d456,5,d457,5,d458,5,d459,5,d460,5,d461,5,d462,5,d463,5,d464,5,d465,5,d466,5,d467,5,d468,5,d469,5,d470,5,d471,5,d472,5,d473,5,d474,5,d475,5,d476,5,d477,5,d478,5,d479,5,d480,5,d481,5,d482,5,d483,5,d484,5,d485,5,d486,5,d487,5,d488,5,d489,5,d490,5,d491,5,d492,5,d493,5,d494,5,d495,5,d496,5,d497,5,d498,5,d499,5,d500,5,d501,5,d502,5,d503,5,d504,5,d505,5,d506,5,d507,5,d508,5,d509,5,d510,5,d511,5,d512,5,d513,5,d514,5,d515,5,d516,5,d517,5,d518,5,d519,5,d520,5,d521,5,d522,5,d523,5,d524,5,d525,5,d526,5,d527,5,d528,5,d529,5,d530,5,d531,5,d532,5,d533,5,d534,5,d535,5,d536,5,d537,5,d538,5,d539,5,d540,5,d541,5,d542,5,d543,5,d544,5,d545,5,d546,5,d547,5,d548,5,d549,5,d550,5,d551,5,d552,5,d553,5,d554,5,d555,5,d556,5,d557,5,d558,5,d559,5,d560,5,d561,5,d562,5,d563,5,d564,5,d565,5,d566,5,d567,5,d568,5,d569,5,d570,5,d571,5,d572,5,d573,5,d574,5,d575,5,d576,5,d577,5,d578,5,d579,5,d580,5,d581,5,d582,5,d583,5,d584,5,d585,5,d586,5,d587,5,d588,5,d589,5,d590,5,d591,5,d592,5,d593,5,d594,5,d595,5,d596,5,d597,5,d598,5,d599,5,d600,5,d601,5,d602,5,d603,5,d604,5,d605,5,d606,5,d607,5,d608,5,d609,5,d610,5,d611,5,d612,5,d613,5,d614,5,d615,5,d616,5,d617,5,d618,5,d619,5,d620,5,d621,5,d622,5,d623,5,d624,5,d625,5,d626,5,d627,5,d628,5,d629,5,d630,5,d631,5,d632,5,d633,5,d634,5,d635,5,d636,5,d637,5,d638,5,d639,5,d640,5,d641,5,d642,5,d643,5,d644,5,d645,5,d646,5,d647,5,d648,5,d649,5,d650,5,d651,5,d652,5,d653,5,d654,5,d655,5,d656,5,d657,5,d658,5,d659,5,d660,5,d661,5,d662,5,d663,5,d664,5,d665,5,d666,5,d667,5,d668,5,d669,5,d670,5,d671,5,d672,5,d673,5,d674,5,d675,5,d676,5,d677,5,d678,5,d679,5,d680,5,d681,5,d682,5,d683,5,d684,5,d685,5,d686,5,d687,5,d688,5,d689,5,d690,5,d691,5,d692,5,d693,5,d694,5,d695,5,d696,5,d697,5,d698,5,d699,5,d700,5,d701,5,d702,5,d703,5,d704,5,d705,5,d706,5,d707,5,d708,5,d709,5,d710,5,d711,5,d712,5,d713,5,d714,5,d715,5,d716,5,d717,5,d718,5,d719,5,d720,5,d721,5,d722,5,d723,5,d724,5,d725,5,d726,5,d727,5,d728,5,d729,5,d730,5,d731,5,d732,5,d733,5,d734,5,d735,5,d736,5,d737,5,d738,5,d739,5,d740,5,d741,5,d742,5,d743,5,d744,5,d745,5,d746,5,d747,5,d748,5,d749,5,d750,5,d751,5,d752,5,d753,5,d754,5,d755,5,d756,5,d757,5,d758,5,d759,5,d760,5,d761,5,d762,5,d763,5,d764,5,d765,5,d766,5,d767,5,d768,5,d769,5,d770,5,d771,5,d772,5,d773,5,d774,5,d775,5,d776,5,d777,5,d778,5,d779,5,d780,5,d781,5,d782,5,d783,5,d784,5,d785,5,d786,5,d787,5,d788,5,d789,5,d790,5,d791,5,d792,5,d793,5,d794,5,d795,5,d796,5,d797,5,d798,5,d799,5,d800,5,d801,5,d802,5,d803,5,d804,5,d805,5,d806,5,d807,5,d808,5,d809,5,d810,5,d811,5,d812,5,d813,5,d814,5,d815,5,d816,5,d817,5,d818,5,d819,5,d820,5,d821,5,d822,5,d823,5,d824,5,d825,5,d826,5,d827,5,d828,5,d829,5,d830,5,d831,5,d832,5,d833,5,d834,5,d835,5,d836,5,d837,5,d838,5,d839,5,d840,5,d841,5,d842,5,d843,5,d844,5,d845,5,d846,5,d847,5,d848,5,d849,5,d850,5,d851,5,d852,5,d853,5,d854,5,d855,5,d856,5,d857,5,d858,5,d859,5,d860,5,d861,5,d862,5,d863,5,d864,5,d865,5,d866,5,d867,5,d868,5,d869,5,d870,5,d871,5,d872,5,d873,5,d874,5,d875,5,d876,5,d877,5,d878,5,d879,5,d880,5,d881,5,d882,5,d883,5,d884,5,d885,5,d886,5,d887,5,d888,5,d889,5,d890,5,d891,5,d892,5,d893,5,d894,5,d895,5,d896,5,d897,5,d898,5,d899,5,d900,5,d901,5,d902,5,d903,5,d904,5,d905,5,d906,5,d907,5,d908,5,d909,5,d910,5,d911,5,d912,5,d913,5,d914,5,d915,5,d916,5,d917,5,d918,5,d919,5,d920,5,d921,5,d922,5,d923,5,d924,5,d925,5,d926,5,d927,5,d928,5,d929,5,d930,5,d931,5,d932,5,d933,5,d934,5,d935,5,d936,5,d937,5,d938,5,d939,5,d940,5,d941,5,d942,5,d943,5,d944,5,d945,5,d946,5,d947,5,d948,5,d949,5,d950,5,d951,5,d952,5,d953,5,d954,5,d955,5,d956,5,d957,5,d958,5,d959,5,d960,5,d961,5,d962,5,d963,5,d964,5,d965,5,d966,5,d967,5,d968,5,d969,5,d970,5,d971,5,d972,5,d973,5,d974,5,d975,5,d976,5,d977,5,d978,5,d979,5,d980,5,d981,5,d982,5,d983,5,d984,5,d985,5,d986,5,d987,5,d988,5,d989,5,d990,5,d991,5,d992,5,d993,5,d994,5,d995,5,d996,5,d997,5,d998,5,d999,5,d1000,5,d1001,5,d1002,5,d1003,5,d1004,5,d1005,5,d1006,5,d1007,5,d1008,5,d1009,5,d1010,5,d1011,5,d1012,5,d1013,5,d1014,5,d1015,5,d1016,5,d1017,5,d1018,5,d1019,5,d1020,5,d1021,5,d1022,5,d1023,5,d1024,5,d1025,5,d1026,5,d1027,5,d1028,5,d1029,5,d1030,5,d1031,5,d1032,5,d1033,5,d1034,5,d1035,5,d1036,5,d1037,5,d1038,5,d1039,5,d1040,5,d1041,5,d1042,5,d1043,5,d1044,5,d1045,5,d1046,5,d1047,5,d1048,5,d1049,5,d1050,5,d1051,5,d1052,5,d1053,5,d1054,5,d1055,5,d1056,5,d1057,5,d1058,5,d1059,5,d1060,5,d1061,5,d1062,5,d1063,5,d1064,5,d1065,5,d1066,5,d1067,5,d1068,5,d1069,5,d1070,5,d1071,5,d1072,5,d1073,5,d1074,5,d1075,5,d1076,5,d1077,5,d1078,5,d1079,5,d1080,5,d1081,5,d1082,5,d1083,5,d1084,5,d1085,5,d1086,5,d1087,5,d1088,5,d1089,5,d1090,5,d1091,5,d1092,5,d1093,5,d1094,5,d1095,5,d1096,5,d1097,5,d1098,5,d1099,5,d1100,5,d1101,5,d1102,5,d1103,5,d1104,5,d1105,5,d1106,5,d1107,5,d1108,5,d1109,5,d1110,5,d1111,5,d1112,5,d1113,5,d1114,5,d1115,5,d1116,5,d1117,5,d1118,5,d1119,5,d1120,5,d1121,5,d1122,5,d1123,5,d1124,5,d1125,5,d1126,5,d1127,5,d1128,5,d1129,5,d1130,5,d1131,5,d1132,5,d1133,5,d1134,5,d1135,5,d1136,5,d1137,5,d1138,5,d1139,5,d1140,5,d1141,5,d1142,5,d1143,5,d1144,5,d1145,5,d1146,5,d1147,5,d1148,5,d1149,5,d1150,5,d1151,5,d1152,5,d1153,5,d1154,5,d1155,5,d1156,5,d1157,5,d1158,5,d1159,5,d1160,5,d1161,5,d1162,5,d1163,5,d1164,5,d1165,5,d1166,5,d1167,5,d1168,5,d1169,5,d1170,5,d1171,5,d1172,5,d1173,5,d1174,5,d1175,5,d1176,5,d1177,5,d1178,5,d1179,5,d1180,5,d1181,5,d1182,5,d1183,5,d1184,5,d1185,5,d1186,5,d1187,5,d1188,5,d1189,5,d1190,5,d1191,5,d1192,5,d1193,5,d1194,5,d1195,5,d1196,5,d1197,5,d1198,5,d1199,5,d1200,5,d1201,5,d1202,5,d1203,5,d1204,5,d1205,5,d1206,5,d1207,5,d1208,5,d1209,5,d1210,5,d1211,5,d1212,5,d1213,5,d1214,5,d1215,5,d1216,5,d1217,5,d1218,5,d1219,5,d1220,5,d1221,5,d1222,5,d1223,5,d1224,5,d1225,5,d1226,5,d1227,5,d1228,5,d1229,5,d1230,5,d1231,5,d1232,5,d1233,5,d1234,5,d1235,5,d1236,5,d1237,5,d1238,5,d1239,5,d1240,5,d1241,5,d1242,5,d1243,5,d1244,5,d1245,5,d1246,5,d1247,5,d1248,5,d1249,5,d1250,5,d1251,5,d1252,5,d1253,5,d1254,5,d1255,5,d1256,5,d1257,5,d1258,5,d1259,5,d1260,5,d1261,5,d1262,5,d1263,5,d1264,5,d1265,5,d1266,5,d1267,5,d1268,5,d1269,5,d1270,5,d1271,5,d1272,5,d1273,5,d1274,5,d1275,5,d1276,5,d1277,5,d1278,5,d1279,5,d1280,5,d1281,5,d1282,5,d1283,5,d1284,5,d1285,5,d1286,5,d1287,5,d1288,5,d1289,5,d1290,5,d1291,5,d1292,5,d1293,5,d1294,5,d1295,5,d1296,5,d1297,5,d1298,5,d1299,5,d1300,5,d1301,5,d1302,5,d1303,5,d1304,5,d1305,5,d1306,5,d1307,5,d1308,5,d1309,5,d1310,5,d1311,5,d1312,5,d1313,5,d1314,5,d1315,5,d1316,5,d1317,5,d1318,5,d1319,5,d1320,5,d1321,5,d1322,5,d1323,5,d1324,5,d1325,5,d1326,5,d1327,5,d1328,5,d1329,5,d1330,5,d1331,5,d1332,5,d1333,5,d1334,5,d1335,5,d1336,5,d1337,5,d1338,5,d1339,5,d1340,5,d1341,5,d1342,5,d1343,5,d1344,5,d1345,5,d1346,5,d1347,5,d1348,5,d1349,5,d1350,5,d1351,5,d1352,5,d1353,5,d1354,5,d1355,5,d1356,5,d1357,5,d1358,5,d1359,5,d1360,5,d1361,5,d1362,5,d1363,5,d1364,5,d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199\S2-1=0.\S2A=0.750367\RMSD=4.896e-09\RMSF=3.134e-06\Dipole=-0.4921359,-0.8740704,0.0559346\PG=C01 [X(C3H6Cl1O1)]\@

QCISD/cc-pVDZ// BHandHLYP 2/cc-pVDZ

QCISD=-652.1683866

CCSD(T)/cc-pVDZ//BHandHLYP/cc-pVDZ

CCSD(T)=-652.1914238

B3LYP/6-311G**

1\1\GINC-G98\PTS\UB3LYP\6-311G(d,p)\C3H6Cl1O1(2)\MATSU\06-Aug-2005\1\#B3LYP/6-311G** SCF=DIRECT GEOM=CHECK GUESS=READ OPT=(TS,CALCF,EF,Z-MATRIX,MAXCYCLES=100) NOSYMM\acetyl radical with CH3Cl\0,2\ClC,1,r1\X,1,1.,2,90.\C,1,r3,3,a2,2,d1,0\O,2,r4,1,a3,3,d2,0\C,2,r5,1,a4,3,d3,0\H,4,r6,1,a5,3,d4,0\H,4,r7,1,a6,3,d5,0\H,4,r8,1,a7,3,d6,0\H,6,r9,2,a8,5,d7,0\H,6,r10,2,a9,5,d8,0\H,6,r11,2,a10,5,d9,0\H,7,r12,4,a11,1,d10,0\H,7,r13,2,a12,5,d11,0\H,6,r14,1,a13,3,d12,0\H,6,r15,2,a14,5,d13,0\H,6,r16,2,a15,5,d14,0\H,6,r17,2,a16,5,d15,0\H,6,r18,2,a17,5,d16,0\H,6,r19,2,a18,5,d17,0\H,6,r20,2,a19,5,d18,0\H,6,r21,2,a20,5,d19,0\H,6,r22,2,a21,5,d20,0\H,6,r23,2,a22,5,d21,0\H,6,r24,2,a23,5,d22,0\H,6,r25,2,a24,5,d23,0\H,6,r26,2,a25,5,d24,0\H,6,r27,2,a26,5,d25,0\H,6,r28,2,a27,5,d26,0\H,6,r29,2,a28,5,d27,0\H,6,r30,2,a29,5,d28,0\H,6,r31,2,a30,5,d29,0\H,6,r32,2,a31,5,d30,0\H,6,r33,2,a32,5,d31,0\H,6,r34,2,a33,5,d32,0\H,6,r35,2,a34,5,d33,0\H,6,r36,2,a35,5,d34,0\H,6,r37,2,a36,5,d35,0\H,6,r38,2,a37,5,d36,0\H,6,r39,2,a38,5,d37,0\H,6,r40,2,a39,5,d38,0\H,6,r41,2,a40,5,d39,0\H,6,r42,2,a41,5,d40,0\H,6,r43,2,a42,5,d41,0\H,6,r44,2,a43,5,d42,0\H,6,r45,2,a44,5,d43,0\H,6,r46,2,a45,5,d44,0\H,6,r47,2,a46,5,d45,0\H,6,r48,2,a47,5,d46,0\H,6,r49,2,a48,5,d47,0\H,6,r50,2,a49,5,d48,0\H,6,r51,2,a50,5,d49,0\H,6,r52,2,a51,5,d50,0\H,6,r53,2,a52,5,d51,0\H,6,r54,2,a53,5,d52,0\H,6,r55,2,a54,5,d53,0\H,6,r56,2,a55,5,d54,0\H,6,r57,2,a56,5,d55,0\H,6,r58,2,a57,5,d56,0\H,6,r59,2,a58,5,d57,0\H,6,r60,2,a59,5,d58,0\H,6,r61,2,a60,5,d59,0\H,6,r62,2,a61,5,d60,0\H,6,r63,2,a62,5,d61,0\H,6,r64,2,a63,5,d62,0\H,6,r65,2,a64,5,d63,0\H,6,r66,2,a65,5,d64,0\H,6,r67,2,a66,5,d65,0\H,6,r68,2,a67,5,d66,0\H,6,r69,2,a68,5,d67,0\H,6,r70,2,a69,5,d68,0\H,6,r71,2,a70,5,d69,0\H,6,r72,2,a71,5,d70,0\H,6,r73,2,a72,5,d71,0\H,6,r74,2,a73,5,d72,0\H,6,r75,2,a74,5,d73,0\H,6,r76,2,a75,5,d74,0\H,6,r77,2,a76,5,d75,0\H,6,r78,2,a77,5,d76,0\H,6,r79,2,a78,5,d77,0\H,6,r80,2,a79,5,d78,0\H,6,r81,2,a80,5,d79,0\H,6,r82,2,a81,5,d80,0\H,6,r83,2,a82,5,d81,0\H,6,r84,2,a83,5,d82,0\H,6,r85,2,a84,5,d83,0\H,6,r86,2,a85,5,d84,0\H,6,r87,2,a86,5,d85,0\H,6,r88,2,a87,5,d86,0\H,6,r89,2,a88,5,d87,0\H,6,r90,2,a89,5,d88,0\H,6,r91,2,a90,5,d89,0\H,6,r92,2,a91,5,d90,0\H,6,r93,2,a92,5,d91,0\H,6,r94,2,a93,5,d92,0\H,6,r95,2,a94,5,d93,0\H,6,r96,2,a95,5,d94,0\H,6,r97,2,a96,5,d95,0\H,6,r98,2,a97,5,d96,0\H,6,r99,2,a98,5,d97,0\H,6,r100,2,a99,5,d98,0\H,6,r101,2,a100,5,d99,0\H,6,r102,2,a101,5,d100,0\H,6,r103,2,a102,5,d101,0\H,6,r104,2,a103,5,d102,0\H,6,r105,2,a104,5,d103,0\H,6,r106,2,a105,5,d104,0\H,6,r107,2,a106,5,d105,0\H,6,r108,2,a107,5,d106,0\H,6,r109,2,a108,5,d107,0\H,6,r110,2,a109,5,d108,0\H,6,r111,2,a110,5,d109,0\H,6,r112,2,a111,5,d110,0\H,6,r113,2,a112,5,d111,0\H,6,r114,2,a113,5,d112,0\H,6,r115,2,a114,5,d113,0\H,6,r116,2,a115,5,d114,0\H,6,r117,2,a116,5,d115,0\H,6,r118,2,a117,5,d116,0\H,6,r119,2,a118,5,d117,0\H,6,r120,2,a119,5,d118,0\H,6,r121,2,a120,5,d119,0\H,6,r122,2,a121,5,d120,0\H,6,r123,2,a122,5,d121,0\H,6,r124,2,a123,5,d122,0\H,6,r125,2,a124,5,d123,0\H,6,r126,2,a125,5,d124,0\H,6,r127,2,a126,5,d125,0\H,6,r128,2,a127,5,d126,0\H,6,r129,2,a128,5,d127,0\H,6,r130,2,a129,5,d128,0\H,6,r131,2,a130,5,d129,0\H,6,r132,2,a131,5,d130,0\H,6,r133,2,a132,5,d131,0\H,6,r134,2,a133,5,d132,0\H,6,r135,2,a134,5,d133,0\H,6,r136,2,a135,5,d134,0\H,6,r137,2,a136,5,d135,0\H,6,r138,2,a137,5,d136,0\H,6,r139,2,a138,5,d137,0\H,6,r140,2,a139,5,d138,0\H,6,r141,2,a140,5,d139,0\H,6,r142,2,a141,5,d140,0\H,6,r143,2,a142,5,d141,0\H,6,r144,2,a143,5,d142,0\H,6,r145,2,a144,5,d143,0\H,6,r146,2,a145,5,d144,0\H,6,r147,2,a146,5,d145,0\H,6,r148,2,a147,5,d146,0\H,6,r149,2,a148,5,d147,0\H,6,r150,2,a149,5,d148,0\H,6,r151,2,a150,5,d149,0\H,6,r152,2,a151,5,d150,0\H,6,r153,2,a152,5,d151,0\H,6,r154,2,a153,5,d152,0\H,6,r155,2,a154,5,d153,0\H,6,r156,2,a155,5,d154,0\H,6,r157,2,a156,5,d155,0\H,6,r158,2,a157,5,d156,0\H,6,r159,2,a158,5,d157,0\H,6,r160,2,a159,5,d158,0\H,6,r161,2,a160,5,d159,0\H,6,r162,2,a161,5,d160,0\H,6,r163,2,a162,5,d161,0\H,6,r164,2,a163,5,d162,0\H,6,r165,2,a164,5,d163,0\H,6,r166,2,a165,5,d164,0\H,6,r167,2,a166,5,d165,0\H,6,r168,2,a167,5,d166,0\H,6,r169,2,a168,5,d167,0\H,6,r170,2,a169,5,d168,0\H,6,r171,2,a170,5,d169,0\H,6,r172,2,a171,5,d170,0\H,6,r173,2,a172,5,d171,0\H,6,r174,2,a173,5,d172,0\H,6,r175,2,a174,5,d173,0\H,6,r176,2,a175,5,d174,0\H,6,r177,2,a176,5,d175,0\H,6,r178,2,a177,5,d176,0\H,6,r179,2,a178,5,d177,0\H,6,r180,2,a179,5,d178,0\H,6,r181,2,a180,5,d179,0\H,6,r182,2,a181,5,d180,0\H,6,r183,2,a182,5,d181,0\H,6,r184,2,a183,5,d182,0\H,6,r185,2,a184,5,d183,0\H,6,r186,2,a185,5,d184,0\H,6,r187,2,a186,5,d185,0\H,6,r188,2,a187,5,d186,0\H,6,r189,2,a188,5,d187,0\H,6,r190,2,a189,5,d188,0\H,6,r191,2,a190,5,d189,0\H,6,r192,2,a191,5,d190,0\H,6,r193,2,a192,5,d191,0\H,6,r194,2,a193,5,d192,0\H,6,r195,2,a194,5,d193,0\H,6,r196,2,a195,5,d194,0\H,6,r197,2,a196,5,d195,0\H,6,r198,2,a197,5,d196,0\H,6,r199,2,a198,5,d197,0\H,6,r200,2,a199,5,d198,0\H,6,r201,2,a200,5,d199,0\H,6,r202,2,a201,5,d200,0\H,6,r203,2,a202,5,d201,0\H,6,r204,2,a203,5,d202,0\H,6,r205,2,a204,5,d203,0\H,6,r206,2,a205,5,d204,0\H,6,r207,2,a206,5,d205,0\H,6,r208,2,a207,5,d206,0\H,6,r209,2,a208,5,d207,0\H,6,r210,2,a209,5,d208,0\H,6,r211,2,a210,5,d209,0\H,6,r212,2,a211,5,d210,0\H,6,r213,2,a212,5,d211,0\H,6,r214,2,a213,5,d212,0\H,6,r215,2,a214,5,d213,0\H,6,r216,2,a215,5,d214,0\H,6,r217,2,a216,5,d215,0\H,6,r218,2,a217,5,d216,0\H,6,r219,2,a218,5,d217,0\H,6,r220,2,a219,5,d218,0\H,6,r221,2,a220,5,d219,0\H,6,r222,2,a221,5,d220,0\H,6,r223,2,a222,5,d221,0\H,6,r224,2,a223,5,d222,0\H,6,r225,2,a224,5,d223,0\H,6,r226,2,a225,5,d224,0\H,6,r227,2,a226,5,d225,0\H,6,r228,2,a227,5,d226,0\H,6,r229,2,a228,5,d227,0\H,6,r230,2,a229,5,d228,0\H,6,r231,2,a230,5,d229,0\H,6,r232,2,a231,5,d230,0\H,6,r233,2,a232,5,d231,0\H,6,r234,2,a233,5,d232,0\H,6,r235,2,a234,5,d233,0\H,6,r236,2,a235,5,d234,0\H,6,r237,2,a236,5,d235,0\H,6,r238,2,a237,5,d236,0\H,6,r239,2,a238,5,d237,0\H,6,r240,2,a239,5,d238,0\H,6,r241,2,a240,5,d239,0\H,6,r242,2,a241,5,d240,0\H,6,r243,2,a242,5,d241,0\H,6,r244,2,a243,5,d242,0\H,6,r245,2,a244,5,d243,0\H,6,r246,2,a245,5,d244,0\H,6,r247,2,a246,5,d245,0\H,6,r248,2,a247,5,d246,0\H,6,r249,2,a248,5,d247,0\H,6,r250,2,a249,5,d248,0\H,6,r251,2,a250,5,d249,0\H,6,r252,2,a251,5,d250,0\H,6,r253,2,a252,5,d251,0\H,6,r254,2,a253,5,d252,0\H,6,r255,2,a254,5,d253,0\H,6,r256,2,a255,5,d254,0\H,6,r257,2,a256,5,d255,0\H,6,r258,2,a257,5,d256,0\H,6,r259,2,a258,5,d257,0\H,6,r260,2,a259,5,d258,0\H,6,r261,2,a260,5,d259,0\H,6,r262,2,a261,5,d260,0\H,6,r263,2,a262,5,d261,0\H,6,r264,2,a263,5,d262,0\H,6,r265,2,a264,5,d263,0\H,6,r266,2,a265,5,d264,0\H,6,r267,2,a266,5,d265,0\H,6,r268,2,a267,5,d266,0\H,6,r269,2,a268,5,d267,0\H,6,r270,2,a269,5,d268,0\H,6,r271,2,a270,5,d269,0\H,6,r272,2,a271,5,d270,0\H,6,r273,2,a272,5,d271,0\H,6,r274,2,a273,5,d272,0\H,6,r275,2,a274,5,d273,0\H,6,r276,2,a275,5,d274,0\H,6,r277,2,a276,5,d275,0\H,6,r278,2,a277,5,d276,0\H,6,r279,2,a278,5,d277,0\H,6,r280,2,a279,5,d278,0\H,6,r281,2,a280,5,d279,0\H,6,r282,2,a281,5,d280,0\H,6,r283,2,a282,5,d281,0\H,6,r284,2,a283,5,d282,0\H,6,r285,2,a284,5,d283,0\H,6,r286,2,a285,5,d284,0\H,6,r287,2,a286,5,d285,0\H,6,r288,2,a287,5,d286,0\H,6,r289,2,a288,5,d287,0\H,6,r290,2,a289,5,d288,0\H,6,r291,2,a290,5,d289,0\H,6,r292,2,a291,5,d290,0\H,6,r293,2,a292,5,d291,0\H,6,r294,2,a293,5,d292,0\H,6,r295,2,a294,5,d293,0\H,6,r296,2,a295,5,d294,0\H,6,r297,2,a296,5,d295,0\H,6,r298,2,a297,5,d296,0\H,6,r299,2,a298,5,d297,0\H,6,r300,2,a299,5,d298,0\H,6,r301,2,a300,5,d299,0\H,6,r302,2,a301,5,d300,0\H,6,r303,2,a302,5,d301,0\H,6,r304,2,a303,5,d302,0\H,6,r305,2,a304,5,d303,0\H,6,r306,2,a305,5,d304,0\H,6,r307,2,a306,5,d305,0\H,6,r308,2,a307,5,d306,0\H,6,r309,2,a308,5,d307,0\H,6,r310,2,a309,5,d308,0\H,6,r311,2,a310,5,d309,0\H,6,r312,2,a311,5,d310,0\H,6,r313,2,a312,5,d311,0\H,6,r314,2,a313,5,d312,0\H,6,r315,2,a314,5,d313,0\H,6,r316,2,a315,5,d314,0\H,6,r317,2,a316,5,d315,0\H,6,r318,2,a317,5,d316,0\H,6,r319,2,a318,5,d317,0\H,6,r320,2,a319,5,d318,0\H,6,r321,2,a320,5,d319,0\H,6,r322,2,a321,5,d320,0\H,6,r323,2,a322,5,d321,0\H,6,r324,2,a323,5,d322,0\H,6,r325,2,a324,5,d323,0\H,6,r326,2,a325,5,d324,0\H,6,r327,2,a326,5,d325,0\H,6,r328,2,a327,5,d326,0\H,6,r329,2,a328,5,d327,0\H,6,r330,2,a329,5,d328,0\H,6,r331,2,a330,5,d329,0\H,6,r332,2,a331,5,d330,0\H,6,r333,2,a332,5,d331,0\H,6,r334,2,a333,5,d332,0\H,6,r335,2,a334,5,d333,0\H,6,r336,2,a335,5,d334,0\H,6,r337,2,a336,5,d335,0\H,6,r338,2,a337,5,d336,0\H,6,r339,2,a338,5,d337,0\H,6,r340,2,a339,5,d338,0\H,6,r341,2,a340,5,d339,0\H,6,r342,2,a341,5,d340,0\H,6,r343,2,a342,5,d341,0\H,6,r344,2,a343,5,d342,0\H,6,r345,2,a344,5,d343,0\H,6,r346,2,a345,5,d344,0\H,6,r347,2,a346,5,d345,0\H,6,r348,2,a347,5,d346,0\H,6,r349,2,a348,5,d347,0\H,6,r350,2,a349,5,d348,0\H,6,r351,2,a350,5,d349,0\H,6,r352,2,a351,5,d350,0\H,6,r353,2,a352,5,d351,0\H,6,r354,2,a353,5,d352,0\H,6,r355,2,a354,5,d353,0\H,6,r356,2,a355,5,d354,0\H,6,r357,2,a356,5,d355,0\H,6,r358,2,a357,5,d356,0\H,6,r359,2,a358,5,d357,0\H,6,r360,2,a359,5,d358,0\H,6,r361,2,a360,5,d359,0\H,6,r362,2,a361,5,d360,0\H,6,r363,2,a362,5,d361,0\H,6,r364,2,a363,5,d362,0\H,6,r365,2,a364,5,d363,0\H,6,r366,2,a365,5,d364,0\H,6,r367,2,a366,5,d365,0\H,6,r368,2,a367,5,d366,0\H,6,r369,2,a368,5,d367,0\H,6,r370,2,a369,5,d368,0\H,6,r371,2,a370,5,d369,0\H,6,r372,2,a371,5,d370,0\H,6,r373,2,a372,5,d371,0\H,6,r374,2,a373,5,d372,0\H,6,r375,2,a374,5,d373,0\H,6,r376,2,a375,5,d374,0\H,6,r377,2,a376,5,d375,0\H,6,r378,2,a377,5,d376,0\H,6,r379,2,a378,5,d377,0\H,6,r380,2,a379,5,d378,0\H,6,r381,2,a380,5,d379,0\H,6,r382,2,a381,5,d380,0\H,6,r383,2,a382,5,d381,0\H,6,r384,2,a383,5,d382,0\H,6,r385,2,a384,5,d383,0\H,6,r386,2,a385,5,d384,0\H,6,r387,2,a386,5,d385,0\H,6,r388,2,a387,5,d386,0\H,6,r389,2,a388,5,d387,0\H,6,r390,2,a389,5,d388,0\H,6,r391,2,a390,5,d389,0\H,6,r392,2,a391,5,d390,0\H,6,r393,2,a392,5,d391,0\H,6,r394,2,a393,5,d392,0\H,6,r395,2,a394,5,d393,0\H,6,r396,2,a395,5,d394,0\H,6,r397,2,a396,5,d395,0\H,6,r398,2,a397,5,d396,0\H,6,r399,2,a398,5,d397,0\H,6,r400,2,a399,5,d398,0\H,6,r401,2,a400,5,d399,0\H,6,r402,2,a401,5,d400,0\H,6,r403,2,a402,5,d401,0\H,6,r404,2,a403,5,d402,0\H,6,r405,2,a404,5,d403,0\H,6,r406,2,a405,5,d404,0\H,6,r407,2,a406,5,d405,0\H,6,r408,2,a407,5,d406,0\H,6,r409,2,a408,5,d407,0\H,6,r410,2,a409,5,d408,0\H,6,r411,2,a410,5,d409,0\H,6,r412,2,a411,5,d410,0\H,6,r413,2,a412,5,d411,0\H,6,r414,2,a413,5,d412,0\H,6,r415,2,a414,5,d413,0\H,6,r416,2,a415,5,d414,0\H,6,r417,2,a416,5,d415,0\H,6,r418,2,a417,5,d416,0\H,6,r419,2,a418,5,d417,0\H,6,r420,2,a419,5,d418,0\H,6,r421,2,a420,5,d419,0\H,6,r422,2,a421,5,d420,0\H,6,r423,2,a422,5,d421,0\H,6,r424,2,a423,5,d422,0\H,6,r425,2,a424,5,d423,0\H,6,r426,2,a425,5,d424,0\H,6,r427,2,a426,5,d425,0\H,6,r428,2,a427,5,d426,0\H,6,r429,2,a428,5,d427,0\H,6,r430,2,a429,5,d428,0\H,6,r431,2,a430,5,d429,0\H,6,r432,2,a431,5,d430,0\H,6,r433,2,a432,5,d431,0\H,6,r434,2,a433,5,d432,0\H,6,r435,2,a434,5,d433,0\H,6,r436,2,a435,5,d434,0\H,6,r437,2,a436,5,d435,0\H,6,r438,2,a437,5,d436,0\H,6,r439,2,a438,5,d437,0\H,6,r440,2,a439,5,d438,0\H,6,r441,2,a440,5,d439,0\H,6,r442,2,a441,5,d440,0\H,6,r443,2,a442,5,d441,0\H,6,r444,2,a443,5,d442,0\H,6,r445,2,a444,5,d443,0\H,6,r446,2,a445,5,d444,0\H,6,r447,2,a446,5,d445,0\H,6,r448,2,a447,5,d446,0\H,6,r449,2,a448,5,d447,0\H,6,r450,2,a449,5,d448,0\H,6,r451,2,a450,5,d449,0\H,6,r452,2,a451,5,d450,0\H,6,r453,2,a452,5,d451,0\H,6,r454,2,a453,5,d452,0\H,6,r455,2,a454,5,d453,0\H,6,r456,2,a455,5,d454,0\H,6,r457,2,a456,5,d455,0\H,6,r458,2,a457,5,d456,0\H,6,r459,2,a458,5,d457,0\H,6,r460,2,a459,5,d458,0\H,6,r461,2,a460,5,d459,0\H,6,r462,2,a461,5,d460,0\H,6,r463,2,a462,5,d461,0\H,6,r464,2,a463,5,d462,0\H,6,r465,2,a464,5,d463,0\H,6,r466,2,a465,5,d464,0\H,6,r467,2,a466,5,d465,0\H,6,r468,2,a467,5,d466,0\H,6,r469,2,a468,5,d467,0\H,6,r470,2,a469,5,d468,0\H,6,r471,2,a470,5,d469,0\H,6,r472,2,a471,5,d470,0\H,6,r473,2,a472,5,d471,0\H,6,r474,2,a473,5,d472,0\H,6,r475,2,a474,5,d473,0\H,6,r476,2,a475,5,d474,0\H,6,r477,2,a476,5,d475,0\H,6,r478,2,a477,5,d476,0\H,6,r479,2,a478,5,d477,0\H,6,r480,2,a479,5,d478,0\H,6,r481,2,a480,5,d479,0\H,6,r482,2,a481,5,d480,0\H,6,r483,2,a482,5,d481,0\H,6,r484,2,a483,5,d482,0\H,6,r485,2,a484,5,d483,0\H,6,r486,2,a485,5,d484,0\H,6,r487,2,a486,5,d485,0\H,6,r488,2,a487,5,d486,0\H,6,r489,2,a488,5,d487,0\H,6,r490,2,a489,5,d488,0\H,6,r491,2,a490,5,d489,0\H,6,r492,2,a491,5,d490,0\H,6,r493,2,a492,5,d491,0\H,6,r494,2,a493,5,d492,0\H,6,r495,2,a494,5,d493,0\H,6,r496,2,a495,5,d494,0\H,6,r497,2,a496,5,d495,0\H,6,r498,2,a497,5,d496,0\H,6,r499,2,a498,5,d497,0\H,6,r500,2,a499,5,d498,0\H,6,r501,2,a500,5,d499,0\H,6,r502,2,a501,5,d500,0\H,6,r503,2,a502,5,d501,0\H,6,r504,2,a503,5,d502,0\H,6,r505,2,a504,5,d503,0\H,6,r506,2,a505,5,d504,0\H,6,r507,2,a506,5,d505,0\H,6,r508,2,a507,5,d506,0\H,6,r509,2,a508,5,d507,0\H,6,r510,2,a509,5,d508,0\H,6,r511,2,a510,5,d509,0\H,6,r512,2,a511,5,d510,0\H,6,r513,2,a512,5,d511,0\H,6,r514,2,a513,5,d512,0\H,6,r515,2,a514,5,d513,0\H,6,r516,2,a515,5,d514,0\H,6,r517,2,a516,5,d515,0\H,6,r518,2,a517,5,d516,0\H,6,r519,2,a518,5,d517,0\H,6,r520,2,a519,5,d518,0\H,6,r521,2,a520,5,d519,0\H,6,r522,2,a521,5,d520,0\H,6,r523,2,a522,5,d521,0\H,6,r524,2,a523,5,d522,0\H,6,r525,2,a524,5,d523,0\H,6,r526,2,a525,5,d524,0\H,6,r527,2,a526,5,d525,0\H,6,r528,2,a527,5,d526,0\H,6,r529,2,a528,5,d527,0\H,6,r530,2,a529,5,d528,0\H,6,r531,2,a530,5,d529,0\H,6,r532,2,a531,5,d530,0\H,6,r533,2,a532,5,d531,0\H,6,r534,2,a533,5,d532,0\H,6,r535,2,a534,5,d533,0\H,6,r536,2,a535,5,d534,0\H,6,r537,2,a536,5,d535,0\H,6,r538,2,a537,5,d536,0\H,6,r539,2,a538,5,d537,0\H,6,r540,2,a539,5,d538,0\H,6,r541,2,a540,5,d539,0\H,6,r542,2,a541,5,d540,0\H,6,r543,2,a542,5,d541,0\H,6,r544,2,a543,5,d542,0\H,6,r545,2,a544,5,d543,0\H,6,r546,2,a545,5,d544,0\H,6,r547,2,a546,5,d545,0\H,6,r548,2,a547,5,d546,0\H,6,r549,2,a548,5,d547,0\H,6,r550,2,a549,5,d548,0\H,

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1\1\GINC-G98\PTS\UBHandHLYP\Gen\C5H10Cl1O1(2)\MATSU\07-Aug-2005\1\#BHANDHLYP/GEN PSEUD
O=READ SCF=(DIRECT,NOVARACC) OPT=(TS,CALCF,EF,Z-MATRIX,MAXCYCLES=100) NOSYMM\ac
etyl radical with i-PrCl\0,2\C\Cl,1,r1\X,1,1,,2,90.\C,1,r3,3,a2,2,d1,0\O,2,r4,1,a3,3,d2,0\C,2,r5,1,a4,3,d3,0\C,4,r6,1,a
5,3,d4,0\C,4,r7,1,a6,3,d5,0\H,4,r8,1,a7,3,d6,0\H,6,r9,2,a8,5,d7,0\H,6,r10,2,a9,5,d8,0\H,6,r11,2,a10,5,d9,0\H,7,r12,4,
a11,1,d10,0\H,7,r13,4,a12,1,d11,0\H,7,r14,4,a13,1,d12,0\H,8,r15,4,a14,1,d13,0\H,8,r16,4,a15,1,d14,0\H,8,r17,4,a16,
1,d15,0\r1=2.14697943\r3=2.16959056\r4=1.17462738\r5=1.49851073\r6=1.5009472\r7=1.50125371\r8=1.082306
1\r9=1.08648235\r10=1.08605285\r11=1.08610078\r12=1.09323\r13=1.08750481\r14=1.08606995\r15=1.09314325
\r16=1.08643671\r17=1.0876334\ a2=91.11725319\ a3=120.53034235\ a4=109.31633725\ a5=104.62341251\ a6=105.
02372021\ a7=97.98871733\ a8=110.44300772\ a9=108.48806825\ a10=108.45157473\ a11=110.05438234\ a12=110.9
6067718\ a13=111.42640607\ a14=110.07686842\ a15=111.52388125\ a16=110.93316692\ d1=180.01611327\ d2=-92.
83911739\ d3=87.16794874\ d4=-98.14543425\ d5=22.06389546\ d6=-19.84116237\ d7=-0.2150098\ d8=-121.934871
01\ d9=121.45738179\ d10=181.81654415\ d11=62.5762319\ d12=-58.30457313\ d13=178.974618\ d14=59.1798698\
d15=-61.91061272\ Version=x86-Linux-G98RevA.9HF=-286.4898209\S2=0.802263\S2-1=0.\S2A=0.750415\RMS
D=3.685e-09\RMSF=9.399e-06\Dipole=-0.0075447,1.0311386,-0.393142\PG=C01 [X(C5H10Cl1O1)]\@\@

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1\1\GINC-G98\PTS\UBHandHLYP\Gen\C6H12Cl1O1(2)\MATSU\19-Aug-2005\1\#BHANDHLYP/GEN PSEUD
O=READ SCF=(DIRECT,NOVARACC) GEOM=MODIFY GUESS=READ OPT=(TS,CALCF,NOEIGENTEST,
Z-MATRIX,MAXCYCLES=100) NOSYMM\acetyl radical with t-BuCl\0,2\ClC,1,r1\X,1,1,,2,90.\C,1,r3,3,a2,2,d1
,0\O,2,r4,1,a3,3,d2,0\C,2,r5,1,a4,3,d3,0\C,4,r6,1,a5,5,d4,0\C,4,r7,1,a6,5,d5,0\C,4,r8,1,a7,5,d6,0\H,6,r9,2,a8,5,d7,0\H,
6,r10,2,a9,5,d8,0\H,6,r11,2,a10,5,d9,0\H,7,r12,4,a11,1,d10,0\H,7,r13,4,a12,1,d11,0\H,7,r14,4,a13,1,d12,0\H,8,r15,4,
a14,1,d13,0\H,8,r16,4,a15,1,d14,0\H,8,r17,4,a16,1,d15,0\H,9,r18,4,a17,1,d16,0\H,9,r19,4,a18,1,d17,0\H,9,r20,4,a19,
1,d18,0\r1=2.16227984\r3=2.18274499\r4=1.17493642\r5=1.49876405\r6=1.50427762\r7=1.50441595\r8=1.50448
41\r9=1.08658217\r10=1.08610105\r11=1.08607933\r12=1.09377712\r13=1.0865329\r14=1.08642059\r15=1.09364
012\r16=1.08681173\r17=1.08669793\r18=1.09375105\r19=1.086494\r20=1.0867609\ a2=89.73567111\ a3=120.643
12186\ a4=109.28271094\ a5=102.84818845\ a6=103.32784596\ a7=103.09145694\ a8=110.50246153\ a9=108.453351
91\ a10=108.45764987\ a11=109.71726892\ a12=111.38028316\ a13=111.32764032\ a14=109.72197396\ a15=111.403
56736\ a16=111.37706882\ a17=109.71141866\ a18=111.32753241\ a19=111.42782068\ d1=180.13249895\ d2=509.02
32617\ d3=689.00420464\ d4=27.98558418\ d5=148.02210928\ d6=268.11256019\ d7=0.04985315\ d8=-121.65951951
\ d9=121.77015297\ d10=180.2673944\ d11=60.81637445\ d12=-60.28051631\ d13=180.10243944\ d14=60.76707519\
\ d15=-62.505858\ d16=179.42311881\ d17=60.05120817\ d18=-61.20424094\ Version=x86-Linux-G98RevA.9\HF=-.32
5.7889862\S2=0.802918\S2=1=0.\S2A=0.750426\RMSD=5.467e-09\RMSF=7.030e-06\Dipole=0.8932387,-0.53741
32,-0.4661939\PG=C01[X(C6H12Cl1O1)]\ \@
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1\1\GINC-G98\PTS\UBHandHLYP\Gen\C3H6Br1O1(2)\MATSU\04-Aug-2005\1\#BHANDHLYP\GEN PSEUDO
=READ SCF=DIRECT GEOM=CHECK GUESS=READ OPT=(TS,READFC,EF,Z-MATRIX,MAXCYCLES=100
) NOSYMM\acetyl radical with CH3Br\0,2\Br\C,1,r1X,1,1.,2,90.\C,1,r3,3,a2,2,d1,0\O,2,r4,1,a3,3,d2,0\C,2,r5,1,a4,
3,d3,0\H,4,r6,1,a5,3,d4,0\H,4,r7,1,a6,3,d5,0\H,4,r8,1,a7,3,d6,0\H,6,r9,2,a8,5,d7,0\H,6,r10,2,a9,5,d8,0\H,6,r11,2,a10,
5,d9,0\r1=2.24045581\r3=2.29998774\r4=1.17407002\r5=1.5005012\r6=1.0792514\r7=1.07925375\r8=1.07907385
\r9=1.08624004\r10=1.08588123\r11=1.08590395\A2=90.05650886\A3=120.1142693\A4=110.31547166\A5=102.736
64412\A6=102.66258579\A7=102.18016419\A8=109.91567944\A9=108.61571414\A10=108.60622888\A1=181.17455
018\A2=86.74759009\A3=266.74601401\A4=149.98166622\A5=29.86230694\A6=-90.05888632\A7=-0.06294921\A8

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=-121.61522101\d9=121.47295499\\Version=x86-Linux-G98RevA.9\\HF=-206.114908\\S2=0.807987\\S2-1=0.\\S2A=0.750434\\RMSD=3.835e-09\\RMSF=3.623e-06\\Dipole=-0.0610135,-1.075147,-0.0374829\\PG=C01 [X(C3H6Br1O1)]\\@

Transition state for bromine transfer reaction from ethyl bromide 3 (X = Br, R = C₂H₅)

BHandHLYP/DZP

1\\1\\GINC-G98\\PTS\\UBHandHLYP\\Gen\\C4H8Br1O1(2)\\MATSU\\04-Aug-2005\\1\\#BHANDHLYP\\GEN PSEUDO=READ SCF=DIRECT OPT=(TS,CALCFC,EF,Z-MATRIX,MAXCYCLES=100) NOSYMM\\acetyl radical with C H3CH2Br\\0,2\\Br\\C,1,r1\\X,1,1.,2,90.\\C,1,r3,3,a2,2,d1,0\\O,2,r4,1,a3,3,d2,0\\C,2,r5,1,a4,3,d3,0\\C,4,r6,1,a5,3,d4,0\\H,4,r7,1,a6,3,d5,0\\H,4,r8,1,a7,3,d6,0\\H,6,r9,2,a8,5,d7,0\\H,6,r10,2,a9,5,d8,0\\H,6,r11,2,a10,5,d9,0\\H,7,r12,4,a11,1,d10,0\\H,7,r13,4,a12,1,d11,0\\H,7,r14,4,a13,1,d12,0\\r1=2.25905822\\r3=2.30724189\\r4=1.17516795\\r5=1.50099362\\r6=1.50111314\\r7=1.08114834\\r8=1.08114825\\r9=1.08641586\\r10=1.08599312\\r11=1.08599245\\r12=1.09299379\\r13=1.08650793\\r14=1.08650798\\a2=90.00129772\\a3=120.30593385\\a4=110.37252584\\a5=107.58119368\\a6=100.0065581\\a7=100.00622\\a8=110.05856959\\a9=108.5964883\\a10=108.59667723\\a11=110.00179885\\a12=111.32964673\\a13=111.32977041\\d1=180.30061787\\d2=-90.00052418\\d3=90.00051343\\d4=89.99175869\\d5=-31.97370393\\d6=211.95687927\\d7=0.00194642\\d8=-121.58524587\\d9=121.58946366\\d10=179.99890206\\d11=60.52173551\\d12=-60.52386984\\Version=x86-Linux-G98RevA.9\\HF=-245.4125677\\S2=0.809785\\S2-1=0.\\S2A=0.750471\\RMSD=6.540e-09\\RMSF=9.037e-07\\Dipole=-0.0000077,0.9574055,-0.26443\\PG=C01 [X(C4H8Br1O1)]\\@

Transition state for bromine transfer reaction from *i*-propyl bromide 3 (X = Br, R = *i*-C₃H₇)

BHandHLYP/DZP

1\\1\\GINC-G98\\PTS\\UBHandHLYP\\Gen\\C5H10Br1O1(2)\\MATSU\\05-Aug-2005\\1\\#BHANDHLYP\\GEN PSEUDO=READ SCF=(DIRECT,NOVARACC) OPT=(TS,CALCFC,EF,Z-MATRIX,MAXCYCLES=100) NOSYMM\\acetyl radical with *i*-PrBr\\0,2\\Br\\C,1,r1\\X,1,1.,2,90.\\C,1,r3,3,a2,2,d1,0\\O,2,r4,1,a3,3,d2,0\\C,2,r5,1,a4,3,d3,0\\C,4,r6,1,a5,3,d4,0\\C,4,r7,1,a6,3,d5,0\\H,4,r8,1,a7,3,d6,0\\H,6,r9,2,a8,5,d7,0\\H,6,r10,2,a9,5,d8,0\\H,6,r11,2,a10,5,d9,0\\H,7,r12,4,a11,1,d10,0\\H,7,r13,4,a12,1,d11,0\\H,7,r14,4,a13,1,d12,0\\H,8,r15,4,a14,1,d13,0\\H,8,r16,4,a15,1,d14,0\\H,8,r17,4,a16,1,d15,0\\r1=2.27999005\\r3=2.31530941\\r4=1.17575312\\r5=1.50137656\\r6=1.5030134\\r7=1.5032463\\r8=1.08271868\\r9=1.08655707\\r10=1.08603868\\r11=1.08607288\\r12=1.09352106\\r13=1.08743917\\r14=1.08600041\\r15=1.09348625\\r16=1.08624309\\r17=1.08752496\\a2=90.86465067\\a3=120.45165706\\a4=110.36092292\\a5=105.36317143\\a6=105.83655025\\a7=97.622223\\a8=110.16871192\\a9=108.58226982\\a10=108.55799916\\a11=109.73830094\\a12=111.12736881\\a13=111.68062914\\a14=109.75387668\\a15=111.73635513\\a16=111.12044376\\d1=180.11006678\\d2=-95.16746835\\d3=84.84599876\\d4=87.21302021\\d5=211.43528792\\d6=-30.62816923\\d7=-0.12412058\\d8=-121.75598678\\d9=121.47801109\\d10=181.93944112\\d11=62.89385329\\d12=-58.30439219\\d13=178.53358684\\d14=58.84487007\\d15=-62.50915899\\Version=x86-Linux-G98RevA.9\\HF=-284.7108904\\S2=0.81144\\S2-1=0.\\S2A=0.750497\\RMSD=7.976e-09\\RMSF=3.650e-06\\Dipole=0.034115,1.0048291,-0.4128381\\PG=C01 [X(C5H10Br1O1)]\\@

Transition state for bromine transfer reaction from *t*-butyl bromide 3 (X = Br, R = *i*-C₄H₉)

BHandHLYP/DZP

1\\1\\GINC-G98\\PTS\\UBHandHLYP\\Gen\\C6H12Br1O1(2)\\MATSU\\05-Aug-2005\\1\\#BHANDHLYP\\GEN PSEUDO=READ SCF=DIRECT OPT=(TS,CALCFC,NOEIGENTEST,Z-MATRIX,MAXCYCLES=100) NOSYMM\\acetyl radical with *t*-BuBr\\0,2\\Br\\C,1,r1\\X,1,1.,2,90.\\C,1,r3,3,a2,2,d1,0\\O,2,r4,1,a3,3,d2,0\\C,2,r5,1,a4,3,d3,0\\C,4,r6,1,a5,3,d4,0\\C,4,r7,1,a6,3,d5,0\\C,4,r8,1,a7,3,d6,0\\H,6,r9,2,a8,5,d7,0\\H,6,r10,2,a9,5,d8,0\\H,6,r11,2,a10,5,d9,0\\H,7,r12,4,a11,1,d10,0\\H,7,r13,4,a12,1,d11,0\\H,7,r14,4,a13,1,d12,0\\H,8,r15,4,a14,1,d13,0\\H,8,r16,4,a15,1,d14,0\\H,8,r17,4,a16,1,d15,0\\H,9,r18,4,a17,1,d16,0\\H,9,r19,4,a18,1,d17,0\\H,9,r20,4,a19,1,d18,0\\r1=2.30466925\\r3=2.32240036\\r4=1.17598222\\r5=1.50161786\\r6=1.50684778\\r7=1.50693734\\r8=1.50680032\\r9=1.08668337\\r10=1.086046\\r11=1.08610396\\r12=1.09403389\\r13=1.0866095\\r14=1.08656507\\r15=1.09400637\\r16=1.08643014\\r17=1.08662047\\r18=1.09409591\\r19=1.08646413\\r20=1.08633757\\a2=90.21867464\\a3=120.5863487\\a4=110.2489\\a5=104.0203307\\a6=103.66056363\\a7=103.44616208\\a8=110.25711256\\a9=108.55923331\\a10=108.51597144\\a11=109.40440846\\a12=111.57623525\\a13=111.56959451\\a14=109.35260041\\a15=111.55039494\\a16=111.62081705\\a17=109.37449778\\a18=111.59154458\\a19=111.53110246\\d1=180.40931795\\d2=89.74587126\\d3=269.63393661\\d4=59.84571419\\d5=179.95661158\\d6=-60.21619354\\d7=-0.28528238\\d8=-121.96329887\\d9=121.32667129\\d10=180.16717902\\d11=60.95941927\\d12=-60.63248172\\d13=179.45502886\\d14=60.2383576\\d15=-61.3195103\\d16=180.35712672\\d17=61.07496606\\d18=-60.36283478\\Version=x86-Linux-G98RevA.9\\HF=-324.009134\\S2=0.812952\\S2-1=0.\\S2A=0.750517\\RMSD=9.060e-09\\RMSF=6.437e-06\\Dipole=-0.010932,-1.0342179,-0.5004178\\PG=C01 [X(C6H12Br1O1)]\\@

Transition state for iodine transfer reaction from methyl iodide 3 (X = I, R = CH₃)

BHandHLYP/DZP

1\1\GINC-G98\PTS\UBHandHLYP\Gen\C3H6I1O1(2)\MATSU\23-Jul-2005\1\#BHANDHLYP\GEN PSEUDO=R
EAD SCF=DIRECT GEOM=CHECK GUESS=READ OPT=(TS,READFC,EF,Z-MATRIX,MAXCYCLES=100) NOSYMM\iodine transfer from CH3I\0,2\IC,1,r1\X,1,1.,2,90.\C,1,r3,3,a2,2,d1,0\O,2,r4,1,a3,3,d2,0\C,2,r5,1,a4,3,d3,
0\H,4,r6,1,a5,3,d4,0\H,4,r7,1,a6,3,d5,0\H,4,r8,1,a7,3,d6,0\H,6,r9,2,a8,5,d7,0\H,6,r10,2,a9,5,d8,0\H,6,r11,2,a10,5,d9,
0\H,7,r12,4,a11,1,d10,0\H,7,r13,4,a12,1,d11,0\H,7,r14,4,a13,1,d12,0\H,8,r15,4,a14,1,d13,0\H,8,r16,4,a15,1,d14,0\H,8,r17,4,a16,1,d15,0\H,8,r18,4,a17,1,d16,0\H,9,r19,4,a18,1,d17,0\H,9,r20,4,a19,1,d18,0\H,9,r21,4,a20,1,d19,0\H,9,r22,4,a21,1,d20,0\H,9,r23,4,a22,1,d21,0\H,9,r24,4,a23,1,d22,0\H,9,r25,4,a24,1,d23,0\H,9,r26,4,a25,1,d24,0\H,9,r27,4,a26,1,d25,0\H,9,r28,4,a27,1,d26,0\H,9,r29,4,a28,1,d27,0\H,9,r30,4,a29,1,d28,0\H,9,r31,4,a30,1,d29,0\H,9,r32,4,a31,1,d30,0\H,9,r33,4,a32,1,d31,0\H,9,r34,4,a33,1,d32,0\H,9,r35,4,a34,1,d33,0\H,9,r36,4,a35,1,d34,0\H,9,r37,4,a36,1,d35,0\H,9,r38,4,a37,1,d36,0\H,9,r39,4,a38,1,d37,0\H,9,r40,4,a39,1,d38,0\H,9,r41,4,a40,1,d39,0\H,9,r42,4,a41,1,d40,0\H,9,r43,4,a42,1,d41,0\H,9,r44,4,a43,1,d42,0\H,9,r45,4,a44,1,d43,0\H,9,r46,4,a45,1,d44,0\H,9,r47,4,a46,1,d45,0\H,9,r48,4,a47,1,d46,0\H,9,r49,4,a48,1,d47,0\H,9,r50,4,a49,1,d48,0\H,9,r51,4,a50,1,d49,0\H,9,r52,4,a51,1,d50,0\H,9,r53,4,a52,1,d51,0\H,9,r54,4,a53,1,d52,0\H,9,r55,4,a54,1,d53,0\H,9,r56,4,a55,1,d54,0\H,9,r57,4,a56,1,d55,0\H,9,r58,4,a57,1,d56,0\H,9,r59,4,a58,1,d57,0\H,9,r60,4,a59,1,d58,0\H,9,r61,4,a60,1,d59,0\H,9,r62,4,a61,1,d60,0\H,9,r63,4,a62,1,d61,0\H,9,r64,4,a63,1,d62,0\H,9,r65,4,a64,1,d63,0\H,9,r66,4,a65,1,d64,0\H,9,r67,4,a66,1,d65,0\H,9,r68,4,a67,1,d66,0\H,9,r69,4,a68,1,d67,0\H,9,r70,4,a69,1,d68,0\H,9,r71,4,a70,1,d69,0\H,9,r72,4,a71,1,d70,0\H,9,r73,4,a72,1,d71,0\H,9,r74,4,a73,1,d72,0\H,9,r75,4,a74,1,d73,0\H,9,r76,4,a75,1,d74,0\H,9,r77,4,a76,1,d75,0\H,9,r78,4,a77,1,d76,0\H,9,r79,4,a78,1,d77,0\H,9,r80,4,a79,1,d78,0\H,9,r81,4,a80,1,d79,0\H,9,r82,4,a81,1,d80,0\H,9,r83,4,a82,1,d81,0\H,9,r84,4,a83,1,d82,0\H,9,r85,4,a84,1,d83,0\H,9,r86,4,a85,1,d84,0\H,9,r87,4,a86,1,d85,0\H,9,r88,4,a87,1,d86,0\H,9,r89,4,a88,1,d87,0\H,9,r90,4,a89,1,d88,0\H,9,r91,4,a90,1,d89,0\H,9,r92,4,a91,1,d90,0\H,9,r93,4,a92,1,d91,0\H,9,r94,4,a93,1,d92,0\H,9,r95,4,a94,1,d93,0\H,9,r96,4,a95,1,d94,0\H,9,r97,4,a96,1,d95,0\H,9,r98,4,a97,1,d96,0\H,9,r99,4,a98,1,d97,0\H,9,r100,4,a99,1,d98,0\H,9,r101,4,a100,1,d99,0\H,9,r102,4,a101,1,d100,0\H,9,r103,4,a102,1,d101,0\H,9,r104,4,a103,1,d102,0\H,9,r105,4,a104,1,d103,0\H,9,r106,4,a105,1,d104,0\H,9,r107,4,a106,1,d105,0\H,9,r108,4,a107,1,d106,0\H,9,r109,4,a108,1,d107,0\H,9,r110,4,a109,1,d108,0\H,9,r111,4,a110,1,d109,0\H,9,r112,4,a111,1,d110,0\H,9,r113,4,a112,1,d111,0\H,9,r114,4,a113,1,d112,0\H,9,r115,4,a114,1,d113,0\H,9,r116,4,a115,1,d114,0\H,9,r117,4,a116,1,d115,0\H,9,r118,4,a117,1,d116,0\H,9,r119,4,a118,1,d117,0\H,9,r120,4,a119,1,d118,0\H,9,r121,4,a120,1,d119,0\H,9,r122,4,a121,1,d120,0\H,9,r123,4,a122,1,d121,0\H,9,r124,4,a123,1,d122,0\H,9,r125,4,a124,1,d123,0\H,9,r126,4,a125,1,d124,0\H,9,r127,4,a126,1,d125,0\H,9,r128,4,a127,1,d126,0\H,9,r129,4,a128,1,d127,0\H,9,r130,4,a129,1,d128,0\H,9,r131,4,a130,1,d129,0\H,9,r132,4,a131,1,d130,0\H,9,r133,4,a132,1,d131,0\H,9,r134,4,a133,1,d132,0\H,9,r135,4,a134,1,d133,0\H,9,r136,4,a135,1,d134,0\H,9,r137,4,a136,1,d135,0\H,9,r138,4,a137,1,d136,0\H,9,r139,4,a138,1,d137,0\H,9,r140,4,a139,1,d138,0\H,9,r141,4,a140,1,d139,0\H,9,r142,4,a141,1,d140,0\H,9,r143,4,a142,1,d141,0\H,9,r144,4,a143,1,d142,0\H,9,r145,4,a144,1,d143,0\H,9,r146,4,a145,1,d144,0\H,9,r147,4,a146,1,d145,0\H,9,r148,4,a147,1,d146,0\H,9,r149,4,a148,1,d147,0\H,9,r150,4,a149,1,d148,0\H,9,r151,4,a150,1,d149,0\H,9,r152,4,a151,1,d150,0\H,9,r153,4,a152,1,d151,0\H,9,r154,4,a153,1,d152,0\H,9,r155,4,a154,1,d153,0\H,9,r156,4,a155,1,d154,0\H,9,r157,4,a156,1,d155,0\H,9,r158,4,a157,1,d156,0\H,9,r159,4,a158,1,d157,0\H,9,r160,4,a159,1,d158,0\H,9,r161,4,a160,1,d159,0\H,9,r162,4,a161,1,d160,0\H,9,r163,4,a162,1,d161,0\H,9,r164,4,a163,1,d162,0\H,9,r165,4,a164,1,d163,0\H,9,r166,4,a165,1,d164,0\H,9,r167,4,a166,1,d165,0\H,9,r168,4,a167,1,d166,0\H,9,r169,4,a168,1,d167,0\H,9,r170,4,a169,1,d168,0\H,9,r171,4,a170,1,d169,0\H,9,r172,4,a171,1,d170,0\H,9,r173,4,a172,1,d171,0\H,9,r174,4,a173,1,d172,0\H,9,r175,4,a174,1,d173,0\H,9,r176,4,a175,1,d174,0\H,9,r177,4,a176,1,d175,0\H,9,r178,4,a177,1,d176,0\H,9,r179,4,a178,1,d177,0\H,9,r180,4,a179,1,d178,0\H,9,r181,4,a180,1,d179,0\H,9,r182,4,a181,1,d180,0\H,9,r183,4,a182,1,d181,0\H,9,r184,4,a183,1,d182,0\H,9,r185,4,a184,1,d183,0\H,9,r186,4,a185,1,d184,0\H,9,r187,4,a186,1,d185,0\H,9,r188,4,a187,1,d186,0\H,9,r189,4,a188,1,d187,0\H,9,r190,4,a189,1,d188,0\H,9,r191,4,a190,1,d189,0\H,9,r192,4,a191,1,d190,0\H,9,r193,4,a192,1,d191,0\H,9,r194,4,a193,1,d192,0\H,9,r195,4,a194,1,d193,0\H,9,r196,4,a195,1,d194,0\H,9,r197,4,a196,1,d195,0\H,9,r198,4,a197,1,d196,0\H,9,r199,4,a198,1,d197,0\H,9,r200,4,a199,1,d198,0\H,9,r201,4,a200,1,d199,0\H,9,r202,4,a201,1,d200,0\H,9,r203,4,a202,1,d201,0\H,9,r204,4,a203,1,d202,0\H,9,r205,4,a204,1,d203,0\H,9,r206,4,a205,1,d204,0\H,9,r207,4,a206,1,d205,0\H,9,r208,4,a207,1,d206,0\H,9,r209,4,a208,1,d207,0\H,9,r210,4,a209,1,d208,0\H,9,r211,4,a210,1,d209,0\H,9,r212,4,a211,1,d210,0\H,9,r213,4,a212,1,d211,0\H,9,r214,4,a213,1,d212,0\H,9,r215,4,a214,1,d213,0\H,9,r216,4,a215,1,d214,0\H,9,r217,4,a216,1,d215,0\H,9,r218,4,a217,1,d216,0\H,9,r219,4,a218,1,d217,0\H,9,r220,4,a219,1,d218,0\H,9,r221,4,a220,1,d219,0\H,9,r222,4,a221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,1,d420,0\H,9,r423,4,a422,1,d421,0\H,9,r424,4,a423,1,d422,0\H,9,r425,4,a424,1,d423,0\H,9,r426,4,a425,1,d424,0\H,9,r427,4,a426,1,d425,0\H,9,r428,4,a427,1,d426,0\H,9,r429,4,a428,1,d427,0\H,9,r430,4,a429,1,d428,0\H,9,r431,4,a430,1,d429,0\H,9,r432,4,a431,1,d430,0\H,9,r433,4,a432,1,d431,0\H,9,r434,4,a433,1,d432,0\H,9,r435,4,a434,1,d433,0\H,9,r436,4,a435,1,d434,0\H,9,r437,4,a436,1,d435,0\H,9,r438,4,a437,1,d436,0\H,9,r439,4,a438,1,d437,0\H,9,r440,4,a439,1,d438,0\H,9,r441,4,a440,1,d439,0\H,9,r442,4,a441,1,d440,0\H,9,r443,4,a442,1,d441,0\H,9,r444,4,a443,1,d442,0\H,9,r445,4,a444,1,d443,0\H,9,r446,4,a445,1,d444,0\H,9,r447,4,a446,1,d445,0\H,9,r448,4,a447,1,d446,0\H,9,r449,4,a448,1,d447,0\H,9,r450,4,a449,1,d448,0\H,9,r451,4,a450,1,d449,0\H,9,r452,4,a451,1,d450,0\H,9,r453,4,a452,1,d451,0\H,9,r454,4,a453,1,d452,0\H,9,r455,4,a454,1,d453,0\H,9,r456,4,a455,1,d454,0\H,9,r457,4,a456,1,d455,0\H,9,r458,4,a457,1,d456,0\H,9,r459,4,a458,1,d457,0\H,9,r460,4,a459,1,d458,0\H,9,r461,4,a460,1,d459,0\H,9,r462,4,a461,1,d460,0\H,9,r463,4,a462,1,d461,0\H,9,r464,4,a463,1,d462,0\H,9,r465,4,a464,1,d463,0\H,9,r466,4,a465,1,d464,0\H,9,r467,4,a466,1,d465,0\H,9,r468,4,a467,1,d466,0\H,9,r469,4,a468,1,d467,0\H,9,r470,4,a469,1,d468,0\H,9,r471,4,a470,1,d469,0\H,9,r472,4,a471,1,d470,0\H,9,r473,4,a472,1,d471,0\H,9,r474,4,a473,1,d472,0\H,9,r475,4,a474,1,d473,0\H,9,r476,4,a475,1,d474,0\H,9,r477,4,a476,1,d475,0\H,9,r478,4,a477,1,d476,0\H,9,r479,4,a478,1,d477,0\H,9,r480,4,a479,1,d478,0\H,9,r481,4,a480,1,d479,0\H,9,r482,4,a481,1,d480,0\H,9,r483,4,a482,1,d481,0\H,9,r484,4,a483,1,d482,0\H,9,r485,4,a484,1,d483,0\H,9,r486,4,a485,1,d484,0\H,9,r487,4,a486,1,d485,0\H,9,r488,4,a487,1,d486,0\H,9,r489,4,a488,1,d487,0\H,9,r490,4,a489,1,d488,0\H,9,r491,4,a490,1,d489,0\H,9,r492,4,a491,1,d490,0\H,9,r493,4,a492,1,d491,0\H,9,r494,4,a493,1,d492,0\H,9,r495,4,a494,1,d493,0\H,9,r496,4,a495,1,d494,0\H,9,r497,4,a496,1,d495,0\H,9,r498,4,a497,1,d496,0\H,9,r499,4,a498,1,d497,0\H,9,r500,4,a499,1,d498,0\H,9,r501,4,a500,1,d499,0\H,9,r502,4,a501,1,d500,0\H,9,r503,4,a502,1,d501,0\H,9,r504,4,a503,1,d502,0\H,9,r505,4,a504,1,d503,0\H,9,r506,4,a505,1,d504,0\H,9,r507,4,a506,1,d505,0\H,9,r508,4,a507,1,d506,0\H,9,r509,4,a508,1,d507,0\H,9,r510,4,a509,1,d508,0\H,9,r511,4,a510,1,d509,0\H,9,r512,4,a511,1,d510,0\H,9,r513,4,a512,1,d511,0\H,9,r514,4,a513,1,d512,0\H,9,r515,4,a514,1,d513,0\H,9,r516,4,a515,1,d514,0\H,9,r517,4,a516,1,d515,0\H,9,r518,4,a517,1,d516,0\H,9,r519,4,a518,1,d517,0\H,9,r520,4,a519,1,d518,0\H,9,r521,4,a520,1,d519,0\H,9,r522,4,a521,1,d520,0\H,9,r523,4,a522,1,d521,0\H,9,r524,4,a523,1,d522,0\H,9,r525,4,a524,1,d523,0\H,9,r526,4,a525,1,d524,0\H,9,r527,4,a526,1,d525,0\H,9,r528,4,a527,1,d526,0\H,9,r529,4,a528,1,d527,0\H,9,r530,4,a529,1,d528,0\H,9,r531,4,a530,1,d529,0\H,9,r532,4,a531,1,d530,0\H,9,r533,4,a532,1,d531,0\H,9,r534,4,a533,1,d532,0\H,9,r535,4,a534,1,d533,0\H,9,r536,4,a535,1,d534,0\H,9,r537,4,a536,1,d535,0\H,9,r538,4,a537,1,d536,0\H,9,r539,4,a538,1,d537,0\H,9,r540,4,a539,1,d538,0\H,9,r541,4,a540,1,d539,0\H,9,r542,4,a541,1,d540,0\H,9,r543,4,a542,1,d541,0\H,9,r544,4,a543,1,d542,0\H,9,r545,4,a544,1,d543,0\H,9,r546,4,a545,1,d544,0\H,9,r547,4,a546,1,d545,0\H,9,r548,4,a547,1,d546,0\H,9,r549,4,a548,1,d547,0\H,9,r550,4,a549,1,d548,0\H,9,r551,4,a550,1,d549,0\H,9,r552,4,a551,1,d550,0\H,9,r553,4,a552,1,d551,0\H,9,r554,4,a553,1,d552,0\H,9,r555,4,a554,1,d553,0\H,9,r556,4,a555,1,d554,0\H,9,r557,4,a556,1,d555,0\H,9,r558,4,a557,1,d556,0\H,9,r559,4,a558,1,d557,0\H,9,r560,4,a559,1,d558,0\H,9,r561,4,a560,1,d559,0\H,9,r562,4,a561,1,d560,0\H,9,r563,4,a562,1,d561,0\H,9,r564,4,a563,1,d562,0\H,9,r565,4

906894\ a7=104.1276614\ a8=110.09236533\ a9=108.69838448\ a10=108.5080395\ a11=109.06228398\ a12=111.7590
0106\ a13=111.79232422\ a14=109.01736818\ a15=111.79589442\ a16=111.81332761\ a17=109.02089814\ a18=111.8
0545161\ a19=111.75792712\ d1=181.23763571\ d2=85.12359439\ d3=264.89684921\ d4=60.69846105\ d5=180.83409
683\ d6=-59.33836308\ d7=-1.15843955\ d8=-122.89598568\ d9=120.31824553\ d10=180.29550444\ d11=61.2199631
4\ d12=-60.62895728\ d13=179.54547362\ d14=60.46775698\ d15=-61.37943073\ d16=180.39074441\ d17=61.279030
7\ d18=-60.48562416\ \Version=x86-Linux-G98RevA.9\ HF=-322.2278432\ S2=0.825548\ S2-1=0.\ S2A=0.750645\ R
MSD=5.887e-09\ RMSF=8.100e-05\ Dipole=-0.097239,-1.0300185,-0.5170838\ PG=C01 [X(C6H12I1O1)]\ \@

Acetyl radical

UHF/6-311G**

HF=-152.3393275#

UHF/DZP

HF=-152.3325819#

MP2/6-311G**

MP2=-152.7993468#

MP2/DZP

MP2=-152.7544193#

MP2/cc-pVDZ

MP2=-152.7452249#

QCISD/6-311G//MP2/6-311G****

QCISD=-152.8237728#

QCISD/DZP//MP2/DZP

QCISD=-152.7815173#

QCISD/cc-pVDZ//MP2/cc-pVDZ

QCISD=-152.7728254#

CCSD(T)/6-311G//MP2/6-311G****

CCSD(T)=-152.8396731#

CCSD(T)/DZP//MP2/DZP

CCSD(T)=-152.7928709#

CCSD(T)/cc-pVDZ//MP2/cc-pVDZ

CCSD(T)=-152.7856565#

BHandHLYP/6-311G**

HF=-153.1346125#

BHandHLYP/DZP

HF=-153.1225667#

B3LYP/6-311G**

HF=-153.2267718#

B3LYP/DZP

HF=-153.2099196#

These data were taken from Supplementary Materials of H. Matsubara and C. H. Schiesser, *Org. Biomol. Chem.*, 2003, **1**, 4335.

BHandHLYP/cc-pVDZ

1\1\GINC-G98\POpt\UBHandHLYP\CC-pVDZ\C2H3O1(2)\MATSU\20-Apr-2006\1\#BHANDHLYP/CC-PVDZ
SCF=DIRECT FREQ GEOM=CHECK GUESS=READ OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSY
MM\acetyl radical\0,2\C\O,1,r1\C,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3,1,a2,2,d2,0\H,3,r4,1,a3,2,d3,0\|r1=1.1723903
3\|r2=1.50494649\|r3=1.09256924\|r4=1.09426697\|a1=128.62411789\|a2=108.64801151\|a3=110.99049148\|d1=121.71
44533\|d2=-121.7165535\|d3=-0.00102484\|Version=x86-Linux-G98RevA.9\HF=-153.1022288\|S2=0.754588\|S2-1=
0.\|S2A=0.750013\|RMSD=6.285e-09\|RMSF=5.097e-05\|Dipole=0.5256646,-0.0000014,-0.8203761\|PG=C01 [X(C2
H3O1)]\|@

QCISD/cc-pVDZ//BHandHLYP/cc-pVDZ

QCISD=-152.7716207

CCSD(T)/cc-pVDZ//BHandHLYP/cc-pVDZ

CCSD(T)=-152.7841721

B3LYP/cc-pVDZ

1\1\GINC-G98\POpt\UB3LYP\CC-pVDZ\C2H3O1(2)\MATSU\20-Apr-2006\1\#B3LYP/CC-PVDZ SCF=DIRECT
FREQ GEOM=CHECK GUESS=READ OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\acetyl rad
ical\0,2\C\O,1,r1\C,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3,1,a2,2,d2,0\H,3,r4,1,a3,2,d3,0\|r1=1.1868541\|r2=1.5146846\|
r3=1.10128569\|r4=1.10354564\|a1=128.19673479\|a2=108.61315932\|a3=111.38979324\|d1=121.91404754\|d2=-121.
91505687\|d3=-0.00051319\|Version=x86-Linux-G98RevA.9\HF=-153.1902221\|S2=0.752423\|S2-1=0.\|S2A=0.7500
04\|RMSD=5.399e-09\|RMSF=4.758e-05\|Dipole=0.5206519,-0.0000007,-0.7483882\|PG=C01 [X(C2H3O1)]\|@

QCISD/cc-pVDZ//B3LYP/cc-pVDZ

QCISD=-152.7727016

CCSD(T)/cc-pVDZ//B3LYP/cc-pVDZ

CCSD(T)=-152.7854493

Methyl radical

UHF/6-311G**

HF=-39.57291#

UHF/DZP

HF=-39.57180#

MP2/6-311G**

MP2=-39.70724#

MP2/DZP

MP2=-39.69730#

MP2/cc-pVDZ

MP2=-39.69064#

QCISD/6-311G//MP2/6-311G****

QCISD=-39.72913#

QCISD/DZP//MP2/DZP

QCISD=-39.71890#

QCISD/cc-pVDZ//MP2/cc-pVDZ

QCISD=-39.71372#

CCSD(T)/6-311G//MP2/6-311G****

CCSD(T)=-39.73221#

CCSD(T)/DZP//MP2/DZP

CCSD(T)=-39.72130#

CCSD(T)/cc-pVDZ//MP2/cc-pVDZ
CCSD(T)=-39.71628#

B3LYP/6-311G**
HF=-39.85376#

B3LYP/DZP
HF=-39.84890#

These data were taken from Supplementary Materials of H. Matsubara, S. M. Horvat and C. H. Schiesser, *Org. Biomol. Chem.*, 2003, **1**, 1199.

BHandHLYP/6-311G**

1\1\GINC-G98\POpt\UBHandHLYP\6-311G(d,p)\C1H3(2)\MATSU\20-Apr-2006\1\#BHANDHLYP/6-311G** SCF=DIRECT FREQ GEOM=CHECK GUESS=READ OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\methyl radical\0,2\C\H,1,r1\H,1,r1,2,a1\H,1,r1,2,a1,3,d1,0\r1=1.07327147\ a1=119.99824307\ d1=179.99216819 \Version=x86-Linux-G98RevA.9\HF=-39.8240572\S2=0.754528\S2-1=0.\S2A=0.75001\RMSD=9.455e-09\RMSE=3.209e-06\Dipole=0.,-0.000037,0.000005\PG=CS [SG(C1H1),X(H2)]\#@

BHandHLYP/DZP

1\1\GINC-G98\POpt\UBHandHLYP\Gen\C1H3(2)\MATSU\25-Aug-2005\1\#BHANDHLYP/GEN PSEUDO=READ SCF=DIRECT FREQ OPT=(CALCF, Z-MATRIX, MAXCYCLES=100) NOSYMM\methyl radical\0,2\C\H,1,r1\H,1,r1,2,a1\H,1,r1,2,a1,3,d1,0\r1=1.07643912\ a1=119.99940405\ d1=180.00000025 \Version=x86-Linux-G98RevA.9\HF=-39.8210462\S2=0.754267\S2-1=0.\S2A=0.750008\RMSD=5.017e-09\RMSE=5.990e-05\Dipole=0.,0.,0.000027\PG=C02V [C2(H1C1),SGV(H2)]\#@

BHandHLYP/cc-pVDZ

1\1\GINC-G98\POpt\UBHandHLYP\CC-pVDZ\C1H3(2)\MATSU\20-Apr-2006\1\#BHANDHLYP/CC-PVDZ SCF=DIRECT FREQ GEOM=CHECK GUESS=READ OPT=(CALCF, Z-MATRIX, MAXCYCLES=100) NOSYMM\methyl radical\0,2\C\H,1,r1\H,1,r1,2,a1\H,1,r1,2,a1,3,d1,0\r1=1.08266591\ a1=119.99989068\ d1=180.00003109 \Version=x86-Linux-G98RevA.9\HF=-39.8115684\S2=0.754723\S2-1=0.\S2A=0.750011\RMSD=1.287e-09\RMSE=4.152e-05\Dipole=0.,0.0000001,0.0000004\PG=CS [SG(C1H1),X(H2)]\#@

QCISD/cc-pVDZ//BHandHLYP/cc-pVDZ
QCISD=-39.71350

CCSD(T)/cc-pVDZ//BHandHLYP/cc-pVDZ
CCSD(T)=-39.71604

B3LYP/cc-pVDZ

1\1\GINC-G98\POpt\UB3LYP\CC-pVDZ\C1H3(2)\MATSU\20-Apr-2006\1\#B3LYP/CC-PVDZ SCF=DIRECT FREQ GEOM=CHECK GUESS=READ OPT=(CALCF, Z-MATRIX, MAXCYCLES=100) NOSYMM\methyl radical\0,2\C\H,1,r1\H,1,r1,2,a1\H,1,r1,2,a1,3,d1,0\r1=1.09065581\ a1=120.00014876\ d1=180.00000248 \Version=x86-Linux-G98RevA.9\HF=-39.8390649\S2=0.753704\S2-1=0.\S2A=0.750007\RMSD=5.911e-09\RMSE=3.638e-05\Dipole=0.,0.,0.0000001\PG=CS [SG(C1H1),X(H2)]\#@

QCISD/cc-pVDZ//B3LYP/cc-pVDZ
QCISD=-39.71373

CCSD(T)/cc-pVDZ//B3LYP/cc-pVDZ
CCSD(T)=-39.71630

Ethyl radical

BHandHLYP/DZP

1\1\GINC-G98\POpt\UBHandHLYP\Gen\C2H5(2)\MATSU\29-Jul-2005\1\#BHANDHLYP/GEN PSEUDO=READ SCF=DIRECT OPT=(CALCF, Z-MATRIX, MAXCYCLES=100) NOSYMM\ethyl radical\0,2\C\C,1,r1\H,1,r2,2,a1\H,1,r2,2,a1,3,d1,0\H,1,r2,2,a1,3,d2,0\H,2,r3,1,a2,3,d3,0\H,2,r3,1,a2,3,d4,0\r1=1.49152407\ r2=1.09039465\ r3=

1.07833637\A1=111.51650217\A2=120.8199367\A3=119.44762092\A4=-119.44824863\A5=85.6242818\A6=-85.60931143\Version=x86-Linux-G98RevA.9\HF=-79.1186585\S2=0.755057\S2-1=0.\S2A=0.750016\RMSE=3.896e-09\RMSEF=1.099e-03\Dipole=0.0596725,0.0000048,-0.1058654\PG=C01 [X(C2H5)]\@

***i*-Propyl radical**

BHandHLYP/DZP

1\1\GINC-G98\POpt\UBHandHLYP\Gen\C3H7(2)\MATSU\30-Jul-2005\1\#BHANDHLYP/GEN PSEUDO=READ SCF=DIRECT OPT=(CALCFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\i-propyl radical\0,2\C\C,1,r1\C,1,r1,2,a1\H,1,r2,2,a2,3,d1,0\H,2,r3,1,a3,3,d2,0\H,2,r4,1,a4,3,d3,0\H,2,r5,1,a5,3,d4,0\H,3,r3,1,a3,2,d2,0\H,3,r4,1,a4,2,d3,0\H,3,r5,1,a5,2,d4,0\A1=1.49218057\A2=1.07803182\A3=1.09353544\A4=1.09351409\A5=1.08687604\A6=120.41192835\A7=119.79591992\A8=111.4440693\A9=111.43732997\A10=111.91055245\A11=179.99174212\A12=-59.20583679\A13=59.25135085\A14=-179.97816791\Version=x86-Linux-G98RevA.9\HF=-118.4172661\S2=0.7558\S2-1=0.\S2A=0.750024\RMSE=5.411e-09\RMSEF=1.308e-05\Dipole=0.0408986,-0.0000451,0.0234154\PG=C01 [X(C3H7)]\@

***t*-Butyl radical**

BHandHLYP/DZP

1\1\GINC-G98\POpt\UBHandHLYP\Gen\C4H9(2)\MATSU\21-Aug-2005\1\#BHANDHLYP/GEN PSEUDO=READ SCF=DIRECT FREQ OPT=(CALCFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\t-butyl radical\0,2\C\C,1,r1\C,1,r1,2,a1\C,1,r1,2,a1,3,d1,0\H,2,r2,1,a2,3,d2,0\H,2,r3,1,a3,3,d3,0\H,2,r4,1,a4,3,d4,0\H,3,r2,1,a2,2,d5,0\H,3,r3,1,a3,2,d6,0\H,3,r4,1,a4,2,d7,0\H,4,r2,1,a2,3,d8,0\H,4,r3,1,a3,3,d9,0\H,4,r4,1,a4,3,d10,0\A1=1.49603838\A2=1.09416719\A3=1.09154214\A4=1.08896627\A5=118.34378848\A6=111.59190427\A7=111.56619379\A8=111.5572329\A9=154.76248432\A10=42.26849798\A11=-77.15716157\A12=163.32430924\A13=77.08402565\A14=-42.3391149\A15=196.57095025\A16=77.33932077\A17=-42.09656135\A18=196.81903077\Version=x86-Linux-G98RevA.9\HF=-157.7162801\S2=0.755649\S2-1=0.\S2A=0.750025\RMSE=7.295e-09\RMSEF=1.392e-03\Dipole=0.0284976,-0.1351111,0.0180942\PG=C01 [X(C4H9)]\@

Methyl chloride

UHF/6-311G**

1\1\GINC-G98\POpt\RHF\6-311G(d,p)\C1H3Cl1\MATSU\22-Aug-2005\1\#HF/6-311G** SCF=DIRECT GEOM=CHECK GUESS=READ FREQ OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\chloromethane\0,1\C\C,1,r1\H,2,r2,1,a1\H,2,r2,1,a1,3,d1,0\H,2,r2,1,a1,3,d2,0\A1=1.78937811\A2=1.07795909\A3=108.17016437\A4=120.00002084\A5=-120.00002057\Version=x86-Linux-G98RevA.9\HF=-499.1307784\RMSE=4.717e-09\RMSEF=3.836e-05\Dipole=-0.0000001,0.,0.9118916\PG=C01 [X(C1H3Cl1)]\@

UHF/DZP

1\1\GINC-G98\POpt\RHF\Gen\C1H3Cl1\MATSU\21-Aug-2005\1\#HF/GEN PSEUDO=READ SCF=DIRECT GEOM=CHECK GUESS=READ FREQ OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\chloromethane\0,1\C\C,1,r1\H,2,r2,1,a1\H,2,r2,1,a1,3,d1,0\H,2,r2,1,a1,3,d2,0\A1=1.78193074\A2=1.07866241\A3=108.3843991\A4=120.00225148\A5=-120.0022227\Version=x86-Linux-G98RevA.9\HF=-54.3420129\RMSE=3.727e-09\RMSEF=6.824e-05\Dipole=-0.000011,0.,0.9059418\PG=C01 [X(C1H3Cl1)]\@

MP2/6-311G**

1\1\GINC-G98\POpt\RMP2-FC\6-311G(d,p)\C1H3Cl1\MATSU\22-Aug-2005\1\#MP2/6-311G** SCF=DIRECT GEOM=CHECK GUESS=READ FREQ=NUMER OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\chloromethane\0,1\C\C,1,r1\H,2,r2,1,a1\H,2,r2,1,a1,3,d1,0\H,2,r2,1,a1,3,d2,0\A1=1.77643587\A2=1.08814775\A3=108.95477528\A4=119.99999879\A5=-119.99999864\Version=x86-Linux-G98RevA.9\HF=-499.1304779\MP2=-499.4262794\RMSE=4.453e-09\RMSEF=2.092e-05\Dipole=0.,0.,0.7710128\PG=C01 [X(C1H3Cl1)]\@

MP2/DZP

1\1\GINC-G98\POpt\RMP2-FC\Gen\C1H3Cl1\MATSU\21-Aug-2005\1\#MP2/GEN PSEUDO=READ SCF=DIRECT GEOM=CHECK GUESS=READ FREQ=NUMER OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\chloromethane\0,1\C\C,1,r1\H,2,r2,1,a1\H,2,r2,1,a1,3,d1,0\H,2,r2,1,a1,3,d2,0\A1=1.77213551\A2=1.08880057\A3=108.99983282\A4=119.99982919\A5=-119.99982575\Version=x86-Linux-G98RevA.9\HF=-54.3417585\MP2=-54.6201023\RMSE=9.404e-09\RMSEF=1.106e-04\Dipole=0.0000008,0.,0.7782247\PG=C01 [X(C1H3Cl1)]\@

MP2/cc-pVDZ

1\1\GINC-G98\POpt\RMP2-FC\CC-pVDZ\C1H3Cl1\MATSU\22-Aug-2005\1\#MP2/CC-PVDZ SCF=DIRECT GEOM=CHECK GUESS=READ FREQ=NUMER OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\chl
oromethane\0,1\Cl\C,1,r1\H,2,r2,1,a1\H,2,r2,1,a1,3,d1,0\H,2,r2,1,a1,3,d2,0\|r1=1.78506784|r2=1.09814074|a1=108
.81586229\d1=119.99999987\d2=-119.99999987\Version=x86-Linux-G98RevA.9\HF=-499.1174812\MP2=-499.40
31534\RMSE=2.906e-09\RMSF=2.619e-06\Dipole=0.,0.,0.7435543\PG=C03V [C3(C1Cl1),3SGV(H1)]\@

QCISD/6-311G/MP2/6-311G****

QCISD=-499.455810

QCISD/DZP//MP2/DZP

QCISD=-54.649702

QCISD/cc-pVDZ//MP2/cc-pVDZ

QCISD=-499.433397

CCSD(T)/6-311G/MP2/6-311G****

CCSD(T)=-499.464065

CCSD(T)/DZP//MP2/DZP

CCSD(T)=-54.656000

CCSD(T)/cc-pVDZ//MP2/cc-pVDZ

CCSD(T)=-499.440286

BHandHLYP/6-311G**

1\1\GINC-G98\POpt\RBHandHLYP\6-311G(d,p)\C1H3Cl1\MATSU\22-Aug-2005\1\#BHANDHLYP/6-311G** S
CF=DIRECT GEOM=CHECK GUESS=READ FREQ OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSYM
M\chloromethane\0,1\Cl\C,1,r1\H,2,r2,1,a1\H,2,r2,1,a1,3,d1,0\H,2,r2,1,a1,3,d2,0\|r1=1.78741521|r2=1.07930797|a
1=108.31583131\d1=119.99887035\d2=-119.99887459\Version=x86-Linux-G98RevA.9\HF=-500.1025439\RMSE
=9.509e-09\RMSF=4.663e-05\Dipole=0.0000016,0.,0.856979\PG=C01 [X(C1H3Cl1)]\@

BHandHLYP/DZP

1\1\GINC-G98\POpt\RBHandHLYP\Gen\C1H3Cl1\MATSU\19-Aug-2005\1\#BHANDHLYP/GEN PSEUDO=RE
AD SCF=DIRECT OPT=(CALCFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\chloromethane\0,1\Cl\C,1,r1\H,
2,r2,1,a1\H,2,r2,1,a1,3,d1,0\H,2,r2,1,a1,3,d2,0\|r1=1.78194756|r2=1.08248491|a1=108.58677895\d1=119.97696171
\d2=-119.97704536\Version=x86-Linux-G98RevA.9\HF=-54.8034876\RMSE=5.210e-09\RMSF=7.810e-05\Dipole
=0.0001253,0.0000001,0.838182\PG=C01 [X(C1H3Cl1)]\@

BHandHLYP/cc-pVDZ

1\1\GINC-G98\POpt\RBHandHLYP\CC-pVDZ\C1H3Cl1\MATSU\20-Apr-2006\1\#BHANDHLYP/CC-PVDZ SC
F=DIRECT GEOM=CHECK GUESS=READ FREQ OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSYM
M\chloromethane\0,1\Cl\C,1,r1\H,2,r2,1,a1\H,2,r2,1,a1,3,d1,0\H,2,r2,1,a1,3,d2,0\|r1=1.78750948|r2=1.08844227|a
1=108.38361267\d1=120.00065139\d2=-120.00065074\Version=x86-Linux-G98RevA.9\HF=-500.0850181\RMSE
=3.612e-09\RMSF=2.799e-06\Dipole=-0.0000118,0.,0.7934911\PG=C01 [X(C1H3Cl1)]\@

QCISD/cc-pVDZ//BHandHLYP/cc-pVDZ

QCISD=-499.433136

CCSD(T)/cc-pVDZ//BHandHLYP/cc-pVDZ

CCSD(T)=-499.439982

B3LYP/6-311G**

1\1\GINC-G98\POpt\RB3LYP\6-311G(d,p)\C1H3Cl1\MATSU\22-Aug-2005\1\#B3LYP/6-311G** SCF=DIRECT
GEOM=CHECK GUESS=READ FREQ OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\chloromet
hane\0,1\Cl\C,1,r1\H,2,r2,1,a1\H,2,r2,1,a1,3,d1,0\H,2,r2,1,a1,3,d2,0\|r1=1.80635893|r2=1.08693851|a1=108.21170
076\d1=119.99858466\d2=-119.99859309\Version=x86-Linux-G98RevA.9\HF=-500.1507152\RMSE=1.006e-09\R
MSF=5.561e-05\Dipole=-0.0000004,0.,0.8379919\PG=C01 [X(C1H3Cl1)]\@

B3LYP/DZP

1\1\GINC-G98\POpt\RB3LYP\Gen\C1H3Cl1\MATSU\21-Aug-2005\1\#B3LYP/GEN PSEUDO=READ SCF=DIR
ECT GEOM=CHECK GUESS=READ FREQ OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\chlor
omethane\0,1\Cl\C,1,r1\H,2,r2,1,a1\H,2,r2,1,a1,3,d1,0\H,2,r2,1,a1,3,d2,0\|r1=1.7997873|r2=1.09117971|a1=108.53
112279\|d1=120.00163038\|d2=-120.00163706\|Version=x86-Linux-G98RevA.9\HF=-54.8766663\RMSD=4.493e-0
9\RMSF=5.583e-06\Dipole=-0.0000241,0.,0.8081272\PG=C01 [X(C1H3Cl1)]\@

B3LYP/cc-pVDZ

1\1\GINC-G98\POpt\RB3LYP\CC-pVDZ\C1H3Cl1\MATSU\20-Apr-2006\1\#B3LYP/CC-PVDZ SCF=DIRECT G
EOM=CHECK GUESS=READ FREQ OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\chlorometha
ne\0,1\Cl\C,1,r1\H,2,r2,1,a1\H,2,r2,1,a1,3,d1,0\H,2,r2,1,a1,3,d2,0\|r1=1.80522011|r2=1.09701985|a1=108.3387220
7\|d1=120.00042271\|d2=-120.00041584\|Version=x86-Linux-G98RevA.9\HF=-500.1285303\RMSD=4.493e-09\RM
SF=4.537e-06\Dipole=-0.0000153,0.,0.7621696\PG=C01 [X(C1H3Cl1)]\@

QCISD/cc-pVDZ//B3LYP/cc-pVDZ

QCISD=-499.433376

CCSD(T)/cc-pVDZ//B3LYP/cc-pVDZ

CCSD(T)=-499.440305

Ethyl chloride

BHandHLYP/DZP

1\1\GINC-G98\POpt\RBHandHLYP\Gen\C2H5Cl1\MATSU\19-Aug-2005\1\#BHANDHLYP/GEN PSEUDO=RE
AD SCF=DIRECT OPT=(CALCFC,Z-MATRIX,MAXCYCLES=100) NOSYMM FREQ\chloroethane\0,1\Cl\C,1,
r1\C,2,r2,1,a1\H,2,r3,1,a2,3,d1,0\H,2,r3,1,a2,3,d2,0\H,3,r4,2,a3,1,d3,0\H,3,r4,2,a3,1,d4,0\H,3,r5,2,a4,1,d5,0\|r1=1.79
570817|r2=1.5143048|r3=1.08347099|r4=1.08624392|r5=1.08927841|a1=111.21513079|a2=106.39177754|a3=110.
92290053|a4=109.45549312\|d1=121.91390628\|d2=-121.91390661\|d3=60.32039205\|d4=-60.32039693\|d5=179.999
99756\|Version=x86-Linux-G98RevA.9\HF=-94.101658\RMSD=6.020e-09\RMSF=2.249e-05\Dipole=0.0847463,0.
0,0.8771744\PG=C01 [X(C2H5Cl1)]\@

i-Propyl chloride

BHandHLYP/DZP

1\1\GINC-G98\POpt\RBHandHLYP\Gen\C3H7Cl1\MATSU\19-Aug-2005\1\#BHANDHLYP/GEN PSEUDO=RE
AD SCF=DIRECT FREQ OPT=(CALCFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\2-chloropropane\0,1\Cl\
C,1,r1\C,2,r2,1,a1\C,2,r2,1,a1,3,d1,0\H,2,r3,1,a2,3,d2,0\H,3,r4,2,a3,1,d3,0\H,3,r4,2,a3,1,d4,0\H,3,r5,2,a4,1,d5,0\H,4,
r6,2,a5,1,d6,0\H,4,r6,2,a5,1,d7,0\H,4,r7,2,a6,1,d8,0\|r1=1.8112948|r2=1.5167051|r3=1.08434567|r4=1.0865007|r5=
1.0892778|r6=1.08649723|r7=1.08927837|a1=109.13351295|a2=104.46909622|a3=110.88857203|a4=109.4882375
5|a5=110.89123906|a6=109.4867454\|d1=124.32661792\|d2=-117.84262305\|d3=62.83595475\|d4=-57.78925621\|d5=
182.47962804\|d6=57.68899098\|d7=-62.945489\|d8=177.40935005\|Version=x86-Linux-G98RevA.9\HF=-133.3994
541\RMSD=3.352e-09\RMSF=3.832e-04\Dipole=0.0271378,0.0514489,0.9080172\PG=C01 [X(C3H7Cl1)]\@

t-Butyl chloride

BHandHLYP/DZP

1\1\GINC-G98\POpt\RBHandHLYP\Gen\C4H9Cl1\MATSU\19-Aug-2005\1\#BHANDHLYP/GEN PSEUDO=RE
AD SCF=DIRECT FREQ OPT=(CALCFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\t-BuCl\0,1\Cl\C,1,r1\C,2
,r2,1,a1\C,2,r2,1,a1,3,d1,0\C,2,r2,1,a1,3,d2,0\H,3,r3,2,a2,1,d3,0\H,3,r3,2,a2,1,d4,0\H,3,r4,2,a3,1,d5,0\H,4,r5,2,a4,1,d
6,0\H,4,r5,2,a4,1,d7,0\H,4,r6,2,a5,1,d8,0\H,5,r7,2,a6,1,d9,0\H,5,r7,2,a6,1,d10,0\H,5,r8,2,a7,1,d11,0\|r1=1.82877845\
r2=1.52076696|r3=1.08628507|r4=1.08941646|r5=1.08625323|r6=1.089379|r7=1.08625323|r8=1.089379|a1=107.2
9386746|a2=110.96169952|a3=109.43443172|a4=110.95342279|a5=109.43047467|a6=110.9534228|a7=109.43047
466\|d1=120.00742933\|d2=-120.00742933\|d3=60.33687236\|d4=-60.33687254\|d5=179.99999992\|d6=60.23945638\|d
7=-60.44163287\|d8=179.88903332\|d9=60.44163297\|d10=-60.23945627\|d11=180.1109668\|Version=x86-Linux-G9
8RevA.9\HF=-172.6963016\RMSD=5.701e-09\RMSF=9.369e-06\Dipole=-0.0001067,0.,0.9229503\PG=C01 [X(C4
H9Cl1)]\@

Methyl bromide

BHandHLYP/DZP

1\1\GINC-G98\POpt\RBHandHLYP\Gen\C1H3Br1\MATSU\18-Aug-2005\1\#BHANDHLYP/GEN PSEUDO=RE
AD SCF=DIRECT OPT=(CALCFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\bromomethane\0,1\Br\C,1,r1\H,
2,r2,1,a1\H,2,r2,1,a1,3,d1,0\H,2,r2,1,a1,3,d2,0\|r1=1.95093035|r2=1.08138521|a1=108.02309209\|d1=119.99834936

\d2=-119.99835451\\Version=x86-Linux-G98RevA.9\\HF=-53.0148468\\RMSD=3.875e-09\\RMSF=1.448e-05\\Dipole=-0.000015,0.,0.802204\\PG=C01 [X(C1H3Br1)]\\@

Ethyl bromide

BHandHLYP/DZP

1\\1\\GINC-G98\\POpt\\RBHandHLYP\\Gen\\C2H5Br1\\MATSU\\18-Aug-2005\\1\\#BHANDHLYP\\GEN PSEUDO=READ SCF=DIRECT OPT=(CALCFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\\bromoethane\\0,1\\Br\\C,1,r1\\C,2,r2,1,a1\\H,2,r3,1,a2,3,d1,0\\H,2,r3,1,a2,3,d2,0\\H,3,r4,2,a3,1,d3,0\\H,3,r4,2,a3,1,d4,0\\H,3,r5,2,a4,1,d5,0\\r1=1.9663871\\r2=1.51444876\\r3=1.08261667\\r4=1.08605972\\r5=1.08988735\\a1=111.64672999\\a2=105.5278768\\a3=111.15442264\\a4=109.19856031\\d1=122.13804155\\d2=-122.13804184\\d3=60.4583608\\d4=-60.45836085\\d5=180.00000005\\Version=x86-Linux-G98RevA.9\\HF=-92.3117593\\RMSD=5.450e-09\\RMSF=2.127e-05\\Dipole=0.0930407,0.,0.8809273\\PG=CS [SG(C2H1Br1),X(H4)]\\@

i-Propyl bromide

BHandHLYP/DZP

1\\1\\GINC-G98\\POpt\\RBHandHLYP\\Gen\\C3H7Br1\\MATSU\\18-Aug-2005\\1\\#BHANDHLYP\\GEN PSEUDO=READ SCF=DIRECT OPT=(CALCFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\\2-bromopropane\\0,1\\Br\\C,1,r1\\C,2,r2,1,a1\\C,2,r2,1,a1,3,d1,0\\H,2,r3,1,a2,3,d2,0\\H,3,r4,2,a3,1,d3,0\\H,3,r4,2,a3,1,d4,0\\H,3,r5,2,a4,1,d5,0\\H,4,r6,2,a5,1,d6,0\\H,4,r6,2,a5,1,d7,0\\H,4,r7,2,a6,1,d8,0\\r1=1.98495666\\r2=1.51676038\\r3=1.08360203\\r4=1.08629074\\r5=1.09012355\\r6=1.0862881\\r7=1.09012776\\a1=109.33461407\\a2=103.32536905\\a3=111.17435615\\a4=109.13122986\\a5=111.18157033\\a6=109.12903847\\d1=124.67562429\\d2=-117.66694963\\d3=63.16782574\\d4=-57.8379252\\d5=182.59454598\\d6=57.72859994\\d7=-63.28840156\\d8=177.28301932\\Version=x86-Linux-G98RevA.9\\HF=-131.6086129\\RMSD=7.139e-09\\RMSF=4.260e-04\\Dipole=0.0303352,0.0579853,0.9374297\\PG=C01 [X(C3H7Br1)]\\@

t-Butyl bromide

BHandHLYP/DZP

1\\1\\GINC-G98\\POpt\\RBHandHLYP\\Gen\\C4H9Br1\\MATSU\\18-Aug-2005\\1\\#BHANDHLYP\\GEN PSEUDO=READ SCF=DIRECT OPT=(CALCFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\\t-BuBr\\0,1\\Br\\C,1,r1\\C,2,r2,1,a1\\C,2,r2,1,a1,3,d1,0\\C,2,r2,1,a1,3,d2,0\\H,3,r3,2,a2,1,d3,0\\H,3,r3,2,a2,1,d4,0\\H,3,r4,2,a3,1,d5,0\\H,4,r5,2,a4,1,d6,0\\H,4,r5,2,a4,1,d7,0\\H,4,r6,2,a5,1,d8,0\\H,5,r7,2,a6,1,d9,0\\H,5,r7,2,a6,1,d10,0\\H,5,r8,2,a7,1,d11,0\\r1=2.00696132\\r2=1.52066558\\r3=1.08605728\\r4=1.09045892\\r5=1.08603174\\r6=1.09042049\\r7=1.08603174\\r8=1.09042049\\a1=107.26072184\\a2=111.28017356\\a3=108.99031582\\a4=111.27761221\\a5=108.98660817\\a6=111.27761221\\a7=108.98660819\\d1=120.0011149\\d2=-120.0011149\\d3=60.56762951\\d4=-60.56762939\\d5=180.00000007\\d6=60.47652491\\d7=-60.6649235\\d8=179.8957021\\d9=60.6649239\\d10=-60.47652449\\d11=180.10429832\\Version=x86-Linux-G98RevA.9\\HF=-170.9046795\\RMSD=2.175e-09\\RMSF=7.436e-06\\Dipole=-0.0000998,0.,0.9699971\\PG=C01 [X(C4H9Br1)]\\@

Methyl iodide

BHandHLYP/DZP

1\\1\\GINC-G98\\POpt\\RBHandHLYP\\Gen\\C1H3I1\\MATSU\\29-Jul-2005\\1\\#BHANDHLYP\\GEN PSEUDO=READ SCF=DIRECT OPT=(CALCFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\\iodomethane\\0,1\\I\\C,1,r1\\H,2,r2,1,a1\\H,2,r2,1,a1,3,d1,0\\H,2,r2,1,a1,3,d2,0\\r1=2.14061658\\r2=1.08086702\\a1=107.80149998\\d1=119.99226807\\d2=-119.99226769\\Version=x86-Linux-G98RevA.9\\HF=-51.2294837\\RMSD=2.994e-09\\RMSF=8.703e-06\\Dipole=0.000212,0.,0.7078097\\PG=C01 [X(C1H3I1)]\\@

Ethyl iodide

BHandHLYP/DZP

1\\1\\GINC-G98\\POpt\\RBHandHLYP\\Gen\\C2H5I1\\MATSU\\29-Jul-2005\\1\\#BHANDHLYP\\GEN PSEUDO=READ SCF=DIRECT OPT=(CALCFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\\iodoethane\\0,1\\I\\C,1,r1\\C,2,r2,1,a1\\H,2,r3,1,a2,3,d1,0\\H,2,r3,1,a2,3,d2,0\\H,3,r4,2,a3,1,d3,0\\H,3,r4,2,a3,1,d4,0\\H,3,r5,2,a4,1,d5,0\\r1=2.1598179\\r2=1.51605645\\r3=1.0822662\\r4=1.08601534\\r5=1.09031688\\a1=112.29177578\\a2=105.00322348\\a3=111.36757237\\a4=109.10619496\\d1=122.35108119\\d2=-122.351078\\d3=60.53605816\\d4=-60.53603959\\d5=180.00000906\\Version=x86-Linux-G98RevA.9\\HF=-90.5246263\\RMSD=3.735e-09\\RMSF=2.193e-05\\Dipole=0.0911133,0.,0.8294012\\PG=C01 [X(C2H5I1)]\\@

i-Propyl iodide

BHandHLYP/DZP

BHandHLYP/DZP

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1\1\GINC-G98\POpt\RBHandHLYP\Gen\C4H9I1\MATSU\29-Jul-2005\1\#BHANDHLYP\GEN PSEUDO=READ
SCF=DIRECT OPT=(CALCF, Z-MATRIX, MAXCYCLES=100) NOSYMM\tt-Bu\0,1\VC,1,r1\C,2,r2,1,a1\C,2,r
2,1,a1,3,d1,0\C,2,r2,1,a1,3,d2,0\H,3,r3,2,a2,1,d3,0\H,3,r3,2,a2,1,d4,0\H,3,r4,2,a3,1,d5,0\H,4,r5,2,a4,1,d6,0\H,4,r5,2,
a4,1,d7,0\H,4,r6,2,a5,1,d8,0\H,5,r7,2,a6,1,d9,0\H,5,r7,2,a6,1,d10,0\H,5,r8,2,a7,1,d11,0\r1=2.21078257\r2=1.521520
77\r3=1.08597265\r4=1.09147655\r5=1.0859453\r6=1.09144445\r7=1.0859453\r8=1.09144445\ a1=107.50142534\ a
2=111.59919691\ a3=108.63177208\ a4=111.61791557\ a5=108.61718104\ a6=111.61791555\ a7=108.61718107\ d1=1
20.00593155\ d2=-120.00593399\ d3=60.78158638\ d4=-60.78158478\ d5=180.00000079\ d6=60.58833525\ d7=-61.00
826332\ d8=179.78639459\ d9=61.00826138\ d10=-60.58833704\ d11=180.21360351\ \Version=x86-Linux-G98RevA.
9\HF=-169.1149183\ RMSD=9.398e-09\ RMSF=1.012e-05\ Dipole=-0.0002823,0,0.9818604\ PG=C01 [X(C4H9I1)]\
\@

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UHF/6-311G**

```
1\1\GINC-G98\POpt\HF\6-311G(d,p)\C2H3Cl1O1\MATSU\22-Aug-2005\1\#HF/6-311G** SCF=DIRECT GEO
M=CHECK GUESS=READ FREQ OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\acetyl chloride\
\0,1\C\O,1,r1\C,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3,1,a2,2,d2,0\H,3,r4,1,a3,2,d3,0\Cl,1,r5,2,a4,3,d4,0\r1=1.1591826
3\r2=1.50056776\r3=1.08314941\r4=1.08110083\r5=1.79535508\ a1=127.79740475\ a2=109.42913767\ a3=108.6783
9333\ a4=119.79623207\ d1=120.82846168\ d2=-120.82845484\ d3=0.00000325\ d4=180.00000037\ \Version=x86-Lin
ux-G98RevA.9\HF=-611.8964251\RMSD=4.359e-09\RMSF=1.841e-05\Dipole=0.9525253,0,-0.7937432\PG=C01
[X(C2H3Cl1O1)]\ \@
```

UHF/DZP

```
1\1\GINC-G98\POpt\RHF\Gen\C2H3Cl1O1\MATSU\21-Aug-2005\1\#HF/GEN PSEUDO=READ SCF=DIRECT
GEOM=CHECK GUESS=READ FREQ OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\acetyl chlo
rode\0,1\C\O,1,r1\C,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3,1,a2,2,d2,0\H,3,r4,1,a3,2,d3,0\Cl,1,r5,2,a4,3,d4,0\r1=1.170
70543\r2=1.50436745\r3=1.08321423\r4=1.08073168\r5=1.77494628\ a1=127.21508556\ a2=109.31424115\ a3=108.
86349223\ a4=120.15113616\ d1=120.89125262\ d2=-120.89152049\ d3=-0.00012929\ d4=179.99997516\ \Version=x8
6-Linux-G98RevA.9\HF=-167.1053932\RMSD=4.305e-09\RMSF=5.814e-06\Dipole=0.8729161,0.,-0.8580139\PG
=C01 [X(C2H3Cl1O1)]\@
```

MP2/6-311G**

```
1\1\GINC-G98\POpt\RMP2-FC\6-311G(d,p)\C2H3Cl1O1\MATSU\22-Aug-2005\1\#MP2/6-311G** SCF=DIRECT GEOM=CHECK GUESS=READ FREQ=NUMER OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSYM M\acetyl chloride\0,1\C\O,1,r1\C,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3,1,a2,2,d2,0\H,3,r4,1,a3,2,d3,0\Cl,1,r5,2,a4,3,d4,0\r1=1.18918768\r2=1.50216829\r3=1.09179663\r4=1.0899512\r5=1.80486365\a1=127.92326954\a2=109.27113262\a3=109.14583643\a4=120.78608482\d1=121.18815537\d2=-121.18790462\d3=0.00011928\d4=180.00002047\Version=x86-Linux-G98RevA.9\HF=-611.8942843\MP2=-612.5170978\RMSE=6.990e-09\RMSF=3.388e-05\Dipole=0.8719178,0,-0.6217824\PG=C01 [X(C2H3Cl1O1)]\@
```

MP2/DZP

```
1\1\GINC-G98\POpt\RMP2-FC\Gen\C2H3Cl1O1\MATSU\21-Aug-2005\1\#MP2/GEN PSEUDO=READ SCF=DI
RECT GEOM=CHECK GUESS=READ FREQ=NUMER OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOS
YMM\acetyl chloride\0,1\C\O,1,r1\C,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3,1,a2,2,d2,0\H,3,r4,1,a3,2,d3,0\Cl,1,r5,2,a4
,3,d4,0\r1=1.20727151\r2=1.50774297\r3=1.09177399\r4=1.08937319\r5=1.78209311\ a1=126.82666173\ a2=109.2
165046\ a3=109.11422267\ a4=120.97616291\ d1=121.09568801\ d2=-121.09391282\ d3=0.0008487\ d4=180.0001365
8\Version=x86-Linux-G98RevA.9\HF=-167.1025802\MP2=-167.6802704\RMSD=3.655e-09\RMSF=4.824e-05\Di
pole=0.7796082,0,-0.7373642\PG=C01 [X(C2H3Cl1O1)]\@
```

MP2/cc-pVDZ

1\1\GINC-G98\POpt\RMP2-FC\CC-pVDZ\C2H3Cl1O1\MATSU\22-Aug-2005\1\#MP2/CC-PVDZ SCF=DIRECT
GEOM=CHECK GUESS=READ FREQ=NUMER OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\acetyl
chloride\0,1\C\O,1,r1\C,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3,1,a2,2,d2,0\H,3,r4,1,a3,2,d3,0\Cl,1,r5,2,a4,3,d4,0\
r1=1.19531284\r2=1.50558168\r3=1.10098712\r4=1.09914588\r5=1.81733322\ a1=128.13412077\ a2=109.2269235
5\ a3=109.27397282\ a4=120.8104469\ d1=121.19758533\ d2=-121.19754652\ d3=0.00001745\ d4=180.00000098\ \Ver
sion=x86-Linux-G98RevA.9\HF=-611.8644796\MP2=-612.4583377\RMSD=4.454e-09\RMSF=9.416e-05\Dipole=0
.8467322,0.,-0.5845592\PG=C01 [X(C2H3Cl1O1)]\@

QCISD/6-311G//MP2/6-311G****

QCISD=-612.546503

QCISD/DZP//MP2/DZP

QCISD=-167.712413

QCISD/cc-pVDZ//MP2/cc-pVDZ

QCISD=-612.490375

CCSD(T)/6-311G//MP2/6-311G****

CCSD(T)=-612.568365

CCSD(T)/DZP//MP2/DZP

CCSD(T)=-167.728970

CCSD(T)/cc-pVDZ//MP2/cc-pVDZ

CCSD(T)=-612.508422

BHandHLYP/6-311G**

1\1\GINC-G98\POpt\RBHandHLYP\6-311G(d,p)\C2H3Cl1O1\MATSU\22-Aug-2005\1\#BHANDHLYP/6-311G*
* SCF=DIRECT GEOM=CHECK GUESS=READ FREQ OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOS
YMM\acetyl chloride\0,1\C\O,1,r1\C,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3,1,a2,2,d2,0\H,3,r4,1,a3,2,d3,0\Cl,1,r5,2,a
4,3,d4,0\r1=1.16714907\r2=1.49237926\r3=1.08402212\r4=1.08185894\r5=1.80817283\ a1=128.18489552\ a2=109.
52407366\ a3=108.92022533\ a4=119.91523018\ d1=121.01236276\ d2=-121.01225094\ d3=0.00004925\ d4=179.9999
9601\ \Version=x86-Linux-G98RevA.9\HF=-613.4089682\RMSD=4.664e-09\RMSF=3.177e-05\Dipole=0.9470286,
0.0000001,-0.7276831\PG=C01 [X(C2H3Cl1O1)]\@

BHandHLYP/DZP

1\1\GINC-G98\POpt\RBHandHLYP\Gen\C2H3Cl1O1\MATSU\19-Aug-2005\1\#BHANDHLYP/GEN PSEUDO=
READ SCF=DIRECT FREQ OPT=(CALCFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\acetyl chloride\0,1\C\
O,1,r1\C,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3,1,a2,2,d2,0\H,3,r4,1,a3,2,d3,0\Cl,1,r5,2,a4,3,d4,0\r1=1.18152764\r2=1.
49896876\r3=1.08632058\r4=1.08378023\r5=1.7847444\ a1=127.456088\ a2=109.33782164\ a3=109.16798255\ a4=1
20.34148013\ d1=121.09566718\ d2=-121.09565968\ d3=0.00000318\ d4=180.00000686\ \Version=x86-Linux-G98Re
vA.9\HF=-168.1049052\RMSD=2.418e-09\RMSF=2.193e-05\Dipole=0.8349751,0.,-0.8170552\PG=C01 [X(C2H3
Cl1O1)]\@

BHandHLYP/cc-pVDZ

1\1\GINC-G98\POpt\RBHandHLYP\CC-pVDZ\C2H3Cl1O1\MATSU\20-Apr-2006\1\#BHANDHLYP/CC-PVDZ
SCF=DIRECT GEOM=CHECK GUESS=READ FREQ OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSY
MM\acetyl chloride\0,1\C\O,1,r1\C,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3,1,a2,2,d2,0\H,3,r4,1,a3,2,d3,0\Cl,1,r5,2,a4,3
,d4,0\r1=1.17335019\r2=1.49296573\r3=1.09220386\r4=1.09003503\r5=1.80561404\ a1=128.00442398\ a2=109.411
2232\ a3=109.07357218\ a4=120.12697637\ d1=121.14751547\ d2=-121.14674411\ d3=0.00036182\ d4=179.99991796
\ \Version=x86-Linux-G98RevA.9\HF=-613.3735599\RMSD=7.281e-09\RMSF=1.030e-04\Dipole=0.8665187,0.000
0012,-0.7049869\PG=C01 [X(C2H3Cl1O1)]\@

QCISD/cc-pVDZ//BHandHLYP/cc-pVDZ

QCISD=-612.489284

CCSD(T)/cc-pVDZ//BHandHLYP/cc-pVDZ

CCSD(T)=-612.506950

B3LYP/6-311G**

1\1\GINC-G98\POpt\RB3LYP\6-311G(d,p)\C2H3Cl1O1\MATSU\22-Aug-2005\1\#B3LYP/6-311G** SCF=DIRECT GEOM=CHECK GUESS=READ FREQ OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\acetyl chloride\0,1\C\O,1,r1\C,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3,1,a2,2,d2,0\H,3,r4,1,a3,2,d3,0\Cl,1,r5,2,a4,3,d4,0\|r1=1.17764105\|r2=1.49991788\|r3=1.09157602\|r4=1.08953841\|r5=1.84736581\|a1=128.79337079\|a2=109.59187749\|a3=109.06566657\|a4=119.8791089\|d1=121.0986313\|d2=-121.09834846\|d3=0.00012854\|d4=180.0000074\|Version=x86-Linux-G98RevA.9\HF=-613.5194701\RMSD=1.984e-09\RMSF=4.374e-05\Dipole=0.9995672,0.0000001,-0.653864\PG=C01 [X(C2H3Cl1O1)]\|@

B3LYP/DZP

1\1\GINC-G98\POpt\RB3LYP\Gen\C2H3Cl1O1\MATSU\21-Aug-2005\1\#B3LYP/GEN PSEUDO=READ SCF=DIRECT GEOM=CHECK GUESS=READ FREQ OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\acetyl chloride\0,1\C\O,1,r1\C,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3,1,a2,2,d2,0\H,3,r4,1,a3,2,d3,0\Cl,1,r5,2,a4,3,d4,0\|r1=1.19403161\|r2=1.50839919\|r3=1.0948626\|r4=1.09243991\|r5=1.81699373\|a1=127.87944884\|a2=109.37077318\|a3=109.35622035\|a4=120.37583752\|d1=121.1898479\|d2=-121.18932915\|d3=0.00023155\|d4=180.0000239\|Version=x86-Linux-G98RevA.9\HF=-168.2376242\RMSD=6.927e-09\RMSF=2.272e-05\Dipole=0.8531095,0.0000002,-0.7637695\PG=C01 [X(C2H3Cl1O1)]\|@

B3LYP/cc-pVDZ

1\1\GINC-G98\POpt\RB3LYP\CC-pVDZ\C2H3Cl1O1\MATSU\20-Apr-2006\1\#B3LYP/CC-PVDZ SCF=DIRECT GEOM=CHECK GUESS=READ FREQ OPT=(READFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\acetyl chloride\0,1\C\O,1,r1\C,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3,1,a2,2,d2,0\H,3,r4,1,a3,2,d3,0\Cl,1,r5,2,a4,3,d4,0\|r1=1.18513171\|r2=1.50155238\|r3=1.10063831\|r4=1.09845366\|r5=1.83985207\|a1=128.44706786\|a2=109.48125996\|a3=109.27965617\|a4=120.17323617\|d1=121.26496265\|d2=-121.2648406\|d3=0.00004688\|d4=179.99996175\|Version=x86-Linux-G98RevA.9\HF=-613.4774678\RMSD=3.351e-09\RMSF=1.156e-04\Dipole=0.8916074,0.0000004,-0.6351984\PG=C01 [X(C2H3Cl1O1)]\|@

QCISD/cc-pVDZ//B3LYP/cc-pVDZ

QCISD=-612.490156

CCSD(T)/cc-pVDZ//B3LYP/cc-pVDZ

CCSD(T)=-612.508158

Acetyl bromide

BHandHLYP/DZP

1\1\GINC-G98\POpt\RBHandHLYP\Gen\C2H3Br1O1\MATSU\19-Aug-2005\1\#BHANDHLYP/GEN PSEUDO=READ SCF=DIRECT FREQ OPT=(CALCFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\acetyl bromide\0,1\C\O,1,r1\C,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3,1,a2,2,d2,0\H,3,r4,1,a3,2,d3,0\Br,1,r5,2,a4,3,d4,0\|r1=1.17950276\|r2=1.49991821\|r3=1.08611205\|r4=1.08458265\|r5=1.97389032\|a1=127.52721513\|a2=109.32079754\|a3=108.97040333\|a4=120.08628059\|d1=121.07497637\|d2=-121.07549652\|d3=-0.00024696\|d4=179.99994683\|Version=x86-Linux-G98RevA.9\HF=-166.3125075\RMSD=7.676e-09\RMSF=3.728e-05\Dipole=0.8797166,0.,-0.7621962\PG=C01 [X(C2H3Br1O1)]\|@

Acetyl iodide

BHandHLYP/DZP

1\1\GINC-G98\POpt\RBHandHLYP\Gen\C2H3I1O1\MATSU\29-Jul-2005\1\#BHANDHLYP/GEN PSEUDO=READ SCF=DIRECT OPT=(CALCFC,Z-MATRIX,MAXCYCLES=100) NOSYMM\acetyl iodide\0,1\C\O,1,r1\C,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3,1,a2,2,d2,0\H,3,r4,1,a3,2,d3,0\I,1,r5,2,a4,3,d4,0\|r1=1.17916538\|r2=1.50200084\|r3=1.08613095\|r4=1.08533119\|r5=2.18974554\|a1=127.09154341\|a2=109.24461885\|a3=108.95345781\|a4=120.04778734\|d1=121.10647936\|d2=-121.10676267\|d3=-0.00013496\|d4=179.99998027\|Version=x86-Linux-G98RevA.9\HF=-164.522789\RMSD=2.468e-09\RMSF=5.583e-06\Dipole=0.8777852,0.,-0.7230541\PG=C01 [X(C2H3I1O1)]\|@