Examples of GRRM Applications

(2016.12.03)

Legend: Applied Chemical System		Reference
H_2O, H_2CO		Chem. Phys. Lett. 381 (2004) 277.
$H_5C_2NO_2$	Glycine	Chemistry Letters 33 (2004) 1372.
$H_5C_2NO_2$	Glycine	Chem. Phys. Lett. 398 (2004) 240.
HCN, $(H_2O)_2$, $H_{12}C_6N_2O_2$		Chem. Phys. Lett. 404 (2005) 95.
H_2CO, H_4C_3	Propyne	J. Phys. Chem. A 109 (2005) 5742.
H_3C_2N	Acetonitrile	J. Phys. Chem. A 109 (2005) 7319.
HC_3N	Cyanoacetylene	Chem. Phys. Lett. 418 (2006) 208.
H_5CN, $H_6C_2NO_2$, H_7C_2NO, $H_6C_2N_2O$		Astrophys. J. 640 (2006) 823.
$H_7C_2NO_2$	Alanine	Chemistry Lett. 35 (2006) 492.
C_{20}		J. Chem. Phys. 124 (2006) 174306.
H_2CO, H_2CO_2, LiCHO, AlCHO, CuCHO, HCO_2Li,		J. Phys. Chem. A 110 (2006) 8933.
$H_{16}O_8$	$(H_2O)_8$	J. Phys. Chem. A 111 (2007) 4527.
H_4C_2O	Acetoaldehyde	J. Phys. Chem. A 111 (2007) 5099.
$H_{10}BC_2N$	$(CH_3)_2NH$-BH_3	Organomet. 26 (2007) 3597.
$H_{17}O_{8+}$	$H^+(H_2O)_8$	J. Phys. Chem. A 111 (2007) 10732.
$H_7C_2^+$, H_9C_3+		Chem. Phys. Lett. 447 (2007) 21.
$H_{10}C_5O_3Ru$	$H_8C_5O_3$–RuH_2	J. Phys. Chem. A 111 (2007) 1368.
H_2S-$(H_2O)_n$ (n=5, 6, 7)		J. Phys. Chem. A 112 (2008) 2963.
$(OH)_2PS_2Cu$-CH_3O_2		J. Phys. Chem. A 112 (2008) 5720.
H_2CO		CHem. Phys. Lett. 460 (2008) 55.
$(H_2O)_n$ (n=2-5)		J. Chem. Phys. 129 (2008) 074315.
H_2CO, H_3C_2N, $H_7C_2NO_2$,		Phys. Scripta 78 (2008) 058122.
$H_4CO_2S_2PCu$		Tetrahedron Lett. 49 (2008) 6841.
RuHCl-BINAP		J. Am. Chem. Soc. 130 (2008) 17228.

H_3CO_3	Chem. Phys. Lett. 469 (2009) 57.
$H^+(H_2O)_n$ (n=5, 6, 7)	J. Compt. Chem. 30 (2009) 952.
H_2CO	J. Phys. Chem. A 113 (2009) 1704.
H_6Si_6	Organomet. 28 (2009) 2218.
$(H_2CO)(H_2O)_{100}$, $Si_6(C_{12}H_{17})_6$	J. Chem. Theoret. Compt. 5 (2009) 2736.
H_9O_4Cl $HCl(H_2O)_4$	Chem. Phys. 358 (2009) 196.
H_2CO	J. Chem. Phys. 130 (2009) 114304.
RuHCl-BINAP	J. Mol. Catalysis A 324 (2010) 133.
$R_2Si=NR$ (R=CH_2Ph, Ph, 1-adamntyl, $SiMe_3$)	New J. Chem. 34 (2010) 1637.
H_6C_6	J. Chem. Theory Comput. 6(2010) 1538.
H_6C_3O	J. Phys. Chem. Lett. 1 (2010) 1841.
O-Si(001)	J. Phys. Chem. C 114 (2010) 15671.
H_2CO-H_2O	J. Phys. Chem. A 114 (2010) 11896.
H_6C_3O	J. Phys. Chem. A 114 (2010) 9864.
H8C4O	Chem. Phys. Chem. 11 (2010) 3883.
R_2CO-R_3PCR_2	J. Chem. Phys. 132 (2010) 241102.
H_6C_6	Chem. Phys. Lett. 503 (2011) 322.
H_2CO, Ar_{38}, C_{20}, $(H_2O)_8$, $H^+(H_2O)_8$	Mol. Sci. 5 (2011) A0042.
$(H_2O)_n$ (n=3-11)	Chem. Science 2 (2011) 686.
I_n^- (n=3, 5, 7)	Compt. Theo. Chem. 973 (2011) 69.
NO_3	J. Phys. Chem. Lett. 2 (2011) 934.
RCO_2H+R_2CO	Angew. Chem. Int. Ed. 50 (2011) 644.
$C_{10}H_8$-O_2	J. Phys. Chem. Lett. 2, (2011) 852.
$H_2C=CH$-$OH+H_2CO+H_2O$	J. Chem. Theory Comput. 7 (2011) 2335.
$HCo(CO)_3+CO+H_2+C_2H_4$	J. Chem. Theory Comput. 8 (2012) 380.
C_3H_6O, $(C_3H_6O)_2$	Phys. Chem. Chem. Phys. 14 (2012) 712.
BCNOS "Progress in Theoretical Chemistry and Physics", 22 (2012) 381, Springer.	
H_2CO, H_6C_3O	Adv. Phys. Chem. 2012 (2012) 268124.
$H_9C_9N_3$ $(H_3C_3N)_3$	J. Phys. Chem. A 112 (2012) 7937.
$H_2O+H_2C=C(H)OH+H_2CO$ in $(H_2O)_{299}$	J. Chem. Theory Comput. 8 (2012) 5058.
H_2CO_2	J. Phys. Chem. Lett. 3 (2012) 1900.
NO_3	J. Chem. Theory Comput. 8 (2012) 2600.
Zr_4H_8, $(C_5Me_4SiMe_3)Zr(CH_2SiMe_3)_3$	Organomet. 32 (2013) 2145.
Pt_n (n=6, 7), Pt_6O, $Pt_6O(N_2O)$, Pt_7O, Pt_7O_2	J. Phys. Chem. A 117 (2013) 1275.

$Na(H_2O)_n$ (n=<8)	Chem. Phys. 419 (2013) 124.
$(NSC=Si)R_6$ (R=H, Me, Ant, Xyl)	J. Am. Chem. Soc. 135 (2013) 10606.
C_6H	J. Chem. Phys. 139 (2013) 224311.
H_2C_2O	J. Phys. Chem. A 117 (2013) 7001.
H_3CNH_2	J. Phys. Chem. A 117 (2013) 5757.
H_4C_3,$H_5C_2NO_2$,$H_6C_3O_2$, $HCo(CO)_3+CO+H_2+C_2H_4$	Phys.Chem.Chem.Phys.15(2013)3683.
$PhCHO+C_6H_9$-$OSiMe_3$	J. Chem. Theory Comput. 9 (2013) 2882.
$PhCHO+C_6H_9$-$OSiMe_3+Eu(H_2O)_8$	J. Am. Chem. Soc. 135 (2013) 13972.
NO_3	J. Chem. Theory Comput. 9 (2013) 893.
H_6C_3O	Z. Phys. Chem.10 (2013) 1524.
H_4C_2, H_6C_3	J. Chem. Theory Comput. 9 (2013) 4116.
H_2CO_2	Chem. Lett. 43 (2014) 93.
$PhCHO+C_4H_3O$-$OSiMe_3+H_2O$	Chem. Asian J. 9 (2014) 305.
H_8C_5O	J. Comput. Chem. 35 (2014) 166.
Terpene	Chemical Science DOI:10.1039 (2014).
H_6C_6	Chem. Lett. 43 (2014) 702.
$H_5C_2NO_2K^+$	Chem.Phys. 440 (2014) 135.
H_5CO_3S	J. Phys. Chem. A 118 (2014) 4019.
C_6N	J. Compt. Chem. 35 (2014) 1568.
H_2COS+H_2O, $H_2COS+2H_2O$	Phys. Chem. Chem. Phys. 16 (2014) 24401.
2,3-disila-1,3-butadiene	Chem. Eur. J. 20 (2014) 9424.
$MeReO_3CH_2N_2$	Organmetallics 33 (2014) 3840.
$(t\text{-}Bu\text{-}C_2O)_2(NPH_2)+BH_3NH_3$	Angew. Chem. 126 (2014) 4721.
$C_{10}H_{10}$, RuHCl-BINAP, $Si_6(C_{12}H_{17})_6$, CH_3CHO,	Bull. Chem. Soc. Jpn 87 (201) 1315.
CH_3NO_2	J. Chem. Phys. 140 (2014) 244310.
H_2NO	J. Chem. Phys. 141 (2014) 154303.
H_2Au_8	J. Chem. Theo. Comput. 10 (2014) 1623.
H_6C_4, $H_6C_5N_2O_2$, $H_6C_9O_2$	J. Phys. Chem. A 118 (2014) 12050.
Glycine Schiff base+Benzyl bromide	J. Phys. Chem. B 118 (2014) 5154.
$NH_2CH_2CH_2CN$	J. Chem. Phys. 142 (2015) 074307.
(12,8)-[4]CC⊃$C_{60}(CH_2)_2NMe$	Chemical Science 6 (2015) 2746.
C_{16}, C_{18}, C_{20}, C_{24}, C_{28}, C_{32}, C_{36}, C_{40}	Chem. Lett. 44 (2015) 712.
$(C_{16})_2$, $(C_{24})_3$, Prism-C_{2n} Sheet (n=6,8,12)	Chem. Phys. Lett. 633 (2015) 120.
C_n Tube (n=3-8, 10, 12, 12, 16, 18, 20)	Chem. Phys. Lett. 635 (2015) 180.
[RuH{(S,S)-$TsNCH(C_6H_5)CH(C_6H_5)NH_2$}(p-cymene)	Chem. Asian J. 10 (2015) 112.

Eu^{3+} complex with DODP J. Am. Chem. Soc. Catalysis 5 (2015) 3731.

CH_3Cl+CN, CH_3Br+CN, CF_3Cl+CN, CF_3Br+CN Chem. Phys. Phys. Chem.16 (2015) 181.

Isopenicillin, HCHO+CH_2=CH-OH, CH_2=CH-O-CH_2CH=CH_2 Int.J.Quant.Chem.115 (2015)258.

H_2CO, H_2CO_2 J. Am. Chem. Soc. 137 (2015) 3433.

Au_5 J. Chem. Phys. 143 (2015) 014301.

RNHCOCHROCOR, RNHCOCHRNRCOR J. Org. Chem. 80 (2015) 5652.

4-aryl-3,4-dihydropyrimidin-2(1H)-one J. Org. Chem. 80 (2015) 6959.

Au_n (n=2-11) J. Phys. Chem. C 119 (2015) 11120.

Serine ($C_3H_7NO_3$) Tetrahedron Lett. 56 (2015) 142.

$C_{2n}H_4$ (n=3-20), C_{2n} (n=24, 30, 36) Chem. Phys. Lett. 639 (2015) 178.

C_6H_6 Bull. Chem. Soc. Jpn, 88 (2015) 1284-1290.

$C_{16}H_4$, $C_{40}H_4$, C_{48}, C_{60}, C_{72}, Wavy Carbons Chem. Phys. Lett. 639 (2015)178-182.

$C_2H_4S^+$ (Ethylene sulfide cation) Chem. Phys. Lett. 641 (2015) 97-103.

Au_5 J. Chem. Phys. 143 (2015) 177102.

C_3H_8, C_3H_7, C_3H_6, C_3H_5, C_3H_4, C_3H_3 Phys. Chem. Chem. Phys. 17 (2015) 27789-27805.

Benzene, naphthalene, phenanthrene,

Anthracene, pyrene Phys. Chem. Chem. Phys. 17 (2015) 22561-22565.

Substituted allyl vinyl ether J. Phys. Chem. A 119 (2015) 11641-11649.

Aceneimide compounds J. Phys. Chem. A 119 (2015) 11479-11487.

Silyl enol ether Fe(II) complexes J. Am. Chem. Soc. 137 (2015) 11085-11094.

$[LiBH_3NH_2]_3$ J. Compt. Chem. 37 (2016) 1259-1264.

NC-CH_3X (X = F, Cl) J. Compt. Chem. 37 (2016) 487-493.

10-P-$3^2$3,7-di(*tert*-butyl)-5-aza-2,8-dioxa-l-phosphabicyclo[3.3.0]octa-2,4,6-triene ACS Catal. 6 (2016) 4859-4870.

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L-serine (HO-CH_2-CH(NH_2)-COOH) Chem. Phys. Lett. 652 (2016) 209-215.

fac-[Re^1(bpy)$(CO)_3(PR_3)]^+$ complex Phys. Chem. Phys. Chem. 18 (2016) 17557-17564.

$(CaCO_3)_n$ (n=2-4) Phys. Chem. Phys. Chem. 18 (2016) 2690-2698.

Alpha-pyrone, coumarine Phys. Chem. Phys. Chem. 18 (2016) 2629-2638.

Allyl vinyl ether J. Chem. Phys. B 120 (2016) 1961-1971.

$Eu^{III}(H_2O)_8$+Trimethylsilyl cyclohexanoate+benzaldehyde Acc. Chem. Res. 49 (2016) 763-773.

$(LiNH_2BH_3)_4$ J. Phys. Chem. A 120 (2016) 145-152.

$ReX(CO)_3$(bpy) (X=Cl, Br, I) J. Chem. Theory Comput. 12 (2016) 2335-2345.

Furan, dibenzofuran	Chem. Lett. Doi:10.1246/cl.160398.
CH_3ICl	Computation 4 (2016) 23.
D-Glucose	J. Chem. Theory Comput. 12 (2016) 5293-5308.

To be continued.