Electronic Supplementary Material (ESI) for Polymer Chemistry.

Electronic Supporting Information

The Effects of Lewis Acid Complexation on Type I Radical Photoinitiators and Implications for Pulsed Laser Polymerization

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1. Theoretical methodology

Standard ab initio molecular orbital theory and density functional theory (DFT) calculations were carried out using Gaussian 09,[1] with the exception of URCCSD(T) calculations, which were performed using Molpro 2012[2] and 2015.[2] Calculations on radicals were performed with an unrestricted wave function except in cases designated with an "RO" prefix where a restricted open-shell wave function was used. Calculations were performed at a high-level of theory, previously shown to predict accurate values for the kinetics and thermodynamics of a wide range of radical reactions.[3-5] Throughout this work, we used a modified version of the 6-31+G(d,p) basis set, which uses the standard 6-31+G(d,p) basis set for first and second row atoms[6-10] and an all electron 6-31G(d) basis set for Zn.[11] For brevity, we refer to this modified basis set as 6-31+G(d,p) henceforth. For improved energy calculations, we also employed the all electron 6-31G(d) basis set for Zn. Geometries of all species were optimised at the M06-2X/6-31+G(d,p) level of theory[12] and frequencies, entropies and thermal corrections were also calculated at this same level and scaled by recommended scaling factors.[13] All geometries were verified as local minima (possessing no imaginary frequencies) or for transition state calculations verified as first-order saddle points (possessing a single imaginary frequency).

Accurate singe-point energies were then calculated using the composite high-level ab initio G3(MP2)-RAD method,[14] in conjunction with an ONIOM inspired approximation for larger systems.[15, 16] Solvation corrections were calculated using the SMD model[17] at M06-2X/6-31+G(d,p), with methyl propanoate (chosen to mimic bulk methyl methacrylate) used as the solvent. For consistency with experiment, toluene, acetonitrile and dichloromethane were used as solvents for benchmarking reactions. For all species in this study full systematic conformational searches (at a resolution of 120°) were performed to ensure global, and not merely local minima were located. Lowest energy conformations were generally selected on the basis of their R(O)MP2/GTMP2Large//M06-2X/6-31+G(d,p) solution-phase free-energies, although if several conformations were close in energy (< 4 kJ mol^{-1}) then improved G3(MP2)-RAD//M06-2X/6-31+G(d,p) solution-phase free-energies were used.

2. UV-Vis data

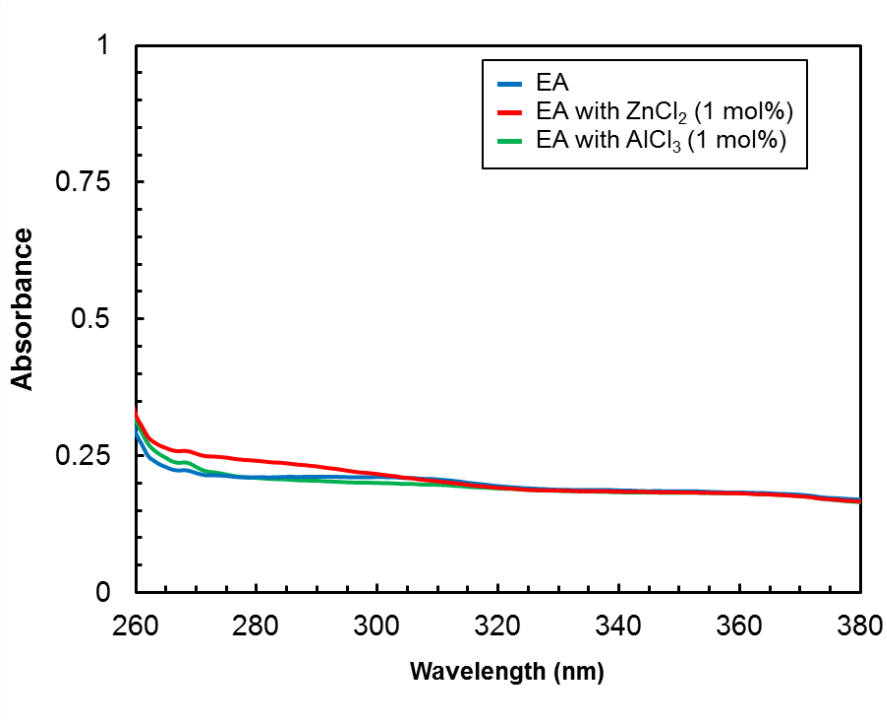


Fig. S1 The negligible absorption of ethyl acetate (EA), and (1 mol%) solutions of $ZnCl_2$ and $AlCl_3$ in EA, in the 260-380 nm range.

Table S1 Summary table of the molar extinction coefficients (ε) of the solutions at different wavelengths.

Photoinitiator System	ε (L mol^{-1} cm^{-1})			
	355 nm	351 nm	325 nm	λmax
MMMP	2.00×10^2	2.55×10^2	3.79×10^3	16.7×10^3
MMMP with $ZnCl_2$ (1 mol%)	2.27×10^3	3.37×10^3	16.4×10^3	16.7×10^3
MMMP with $AlCl_3$ (1 mol%)	2.52×10^3	4.18×10^3	18 .9$\times 10^3$	18.9×10^3
DMPA	1.77×10^2	1.91×10^2	1.84×10^2	6.94×10^3 at 260 nm
DMPA with $ZnCl_2$ (1 mol%)	1.76×10^3	1.95×10^3	3.87×10^3	7.71×10^3 at 260 nm
DMPA with $AlCl_3$ (1 mol%)	1.15×10^3	1.35×10^3	2.46×10^3	21.3×10^3 at 260 nm

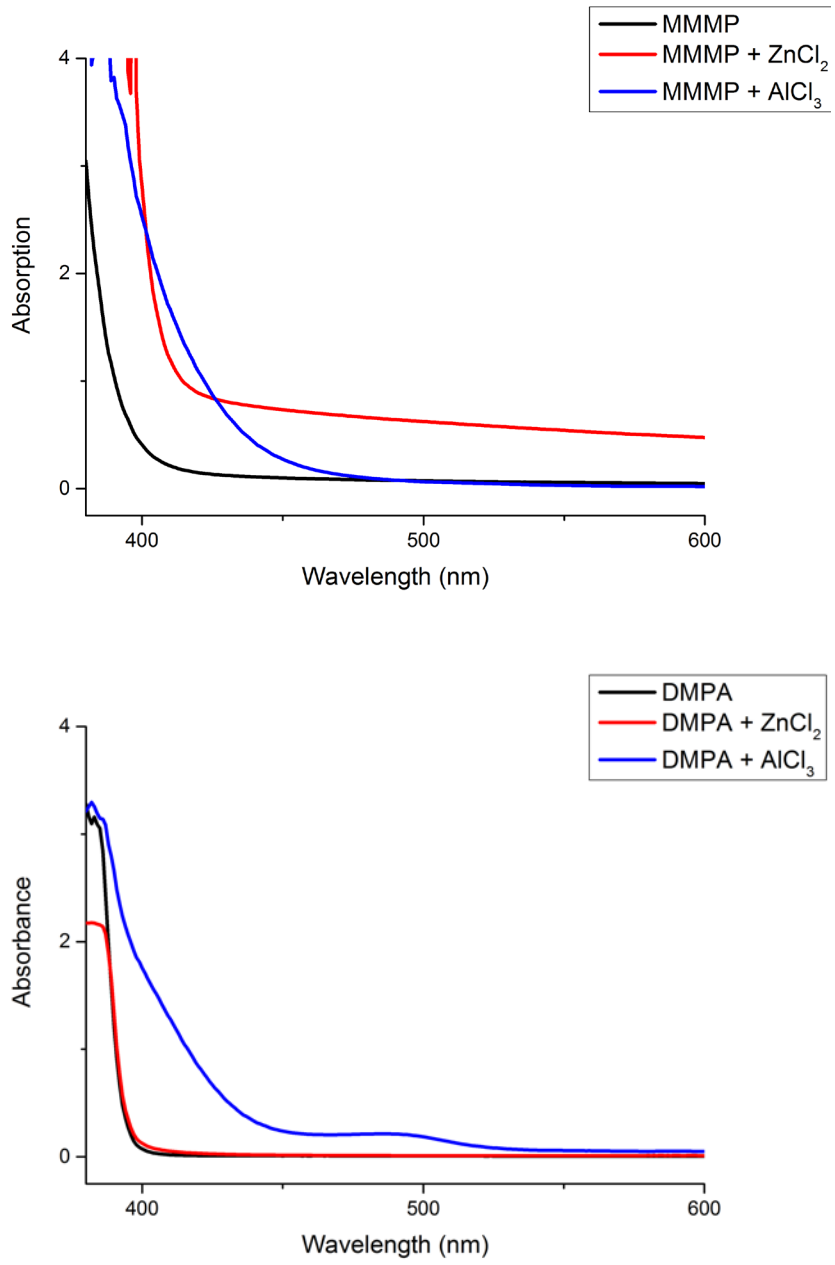


Fig. S2 Visible spectra of the solutions of the photoinitiator (0.15M) with and without Lewis acid (0.15M) in ethyl acetate, showing significant absorption tails in the visible region for the combinations: $AlCl_3$/MMMP, $ZnCl_2$/MMMP and $AlCl_3$/DMPA.

3. General Benchmarking

3.1 Binding Enthalpies

To assess the theoretical methodology used in this study for Lewis acid/base interactions, we benchmarked theoretically predicted binding enthalpies (ΔH_{bind}) against corresponding experimentally derived values for various monodentate [BF_3(Ligand)] complexes (see Table S2). These ligands include a variety of different neutral O and N bases; including ketones, esters, amines and ethers. All experimental values were taken from reference [18]. Unfortunately, a direct evaluation of the computational methodology using these experimental values is slightly problematic. Elsewhere in this work, Gibbs free energies in solution are computed using a Hess's Law thermocycle and gas-phase free-energies in conjunction with free-energies of solvation calculated with SMD (see Theoretical Methodology section above for details). The reliability and accuracy of this thermocycle approach has been confirmed for pK_a values, redox potentials, equilibrium constants and rate coefficients.[3-5] Unfortunately, the SMD model was only parameterized for use at 25 °C and so cannot calculate enthalpies of solvation. This makes it difficult to directly assess the methodological approach employed in this work against experimentally derived solution-phase binding enthalpies. Given these complexities, we used two different theoretically predicted quantities for benchmarking (see **Table S2**).

First, we compared calculated gas-phase binding enthalpies against corresponding solution-phase experimental data. Unsurprisingly, the absolute gas-phase binding enthalpies systematically underestimate the solution-phase complexation enthalpy of every ligand in the test set. Much better agreement is obtained between the relative binding enthalpies, using the [$BF_3(OEt_2)$] complexation reaction as a reference. With this relative approach, a mean absolute deviation (MAD) and a maximum deviation (MAX) of 5.2 and 15.7 kJ mol^{-1}, respectively, were obtained. While reasonable agreement was noted, unfortunately, several ligands had unacceptably large deviations, which almost certainly results from neglect of enthalpic solvation effects. Indeed, the largest deviations from experiment were observed for N,N-dimethylformamide, dimethyl sulfoxide, acetonitrile and propylene carbonate, which all have large permanent dipole moments (> 3.5 D) and hence would be anticipated to have large solvation corrections.

Table S2 Theoretically predicted and experimentally determined binding enthalpies (ΔH_{bind})[a] for various monodentate [BF_3(Ligand)] complexes.

Ligand	Theory: Gas-phase		Theory: Solution-phase		Experiment	
	ΔH_{bind}	ΔH_{bind}(rel)	ΔH_{bind}	ΔH_{bind}(rel)	ΔH_{bind}	ΔH_{bind}(rel)
nitrobenzene	−19.7	39.0	−36.5	42.3	−35.8	43.0
nitromethane	−19.6	39.1	−38.0	40.8	−37.6	41.1
acetonitrile	−26.3	32.4	−55.3	23.5	−60.4	18.4
propylene carbonate	−35.2	23.5	−61.4	17.4	−64.2	14.6
methyl acetate	−51.7	7.0	−69.9	8.9	−72.8	6.0
acetophenone	−51.7	7.0	−72.2	6.6	−74.5	4.3
ethyl acetate	−53.9	4.9	−73.8	8.4	−75.6	3.2
acetone	−51.4	7.3	−73.6	5.2	−76.0	2.7
diethyl ether (*Reference*)	−58.7	0.0[b]	−78.8[b]	0.0[b]	−78.8	0.0[b]
tetrahydropyran	−69.8	−11.1	−88.8	−10.0	−85.4	−6.6
tetrahydrofuran	−73.5	−14.8	−95.3	−16.5	−90.4	−11.6
isophorone	−66.1	−7.4	−90.2	−11.4	−90.6	−11.8
2,4,6-trimethylpyridine	−84.3	−25.6	−99.8	−21.0	−101.0	−22.3
dimethyl sulfoxide	−76.1	−17.4	−107.2	−28.3	−105.3	−26.5
tetramethylurea	−83.9	−25.2	−112.6	−33.8	−108.6	−29.8
N,N-dimethylformamide	−74.7	−16.0	−112.8	−34.0	−110.5	−31.7
pyridine	−99.6	−40.9	−124.4	−45.6	−128.1	−49.3
triethylamine	−120.7	−62.0	−137.0	−58.2	−135.9	−57.1

[a]Theoretical binding enthalpies were calculated at 25 °C. Both experimental and theoretical values are given in kJ mol^{-1}. [b]By definition, as the [$BF_3(OEt_2)$] complexation reaction was used as a reference.

In our second approach, we accounted for the effect of solvation by estimating the solvation enthalpy correction for each complexation reaction. These corrections were approximated by calculating the corresponding solvation free-energy correction (using SMD) and then subtracting an entropic solvation component, which was assumed to be constant for all complexation reactions. That is, the second approach assumes that each BF_3 complexation reaction has the same entropic solvation correction; the value of which is determined by using the [$BF_3(OEt_2)$] reaction as a reference. This approximation should be reasonable because of the inherent similarity of these [BF_3(Ligand)] complexation reactions and the consistent use dichloromethane as a solvent. Moreover, it should be noted that the reported accuracy of most continuum solvation models is only around 4 kJ mol^{-1} for neutral solutes. Provided that variation in the actual entropic solvation corrections is not significantly

greater than 4 kJ mol^{-1}, errors introduced by assuming this correction is constant will be comparable with errors introduced by the continuum solvent model itself. Satisfyingly, excellent quantitative agreement with experimental values was noted using this approach; a MAD and MAX of 2.4 and 5.1 kJ mol^{-1}, respectively, were obtained. This excellent agreement is also illustrated in **Fig. S3**. The close agreement between these theoretical values and experiment, notwithstanding the approximations employed, confirms the accuracy of the theoretical methodology.

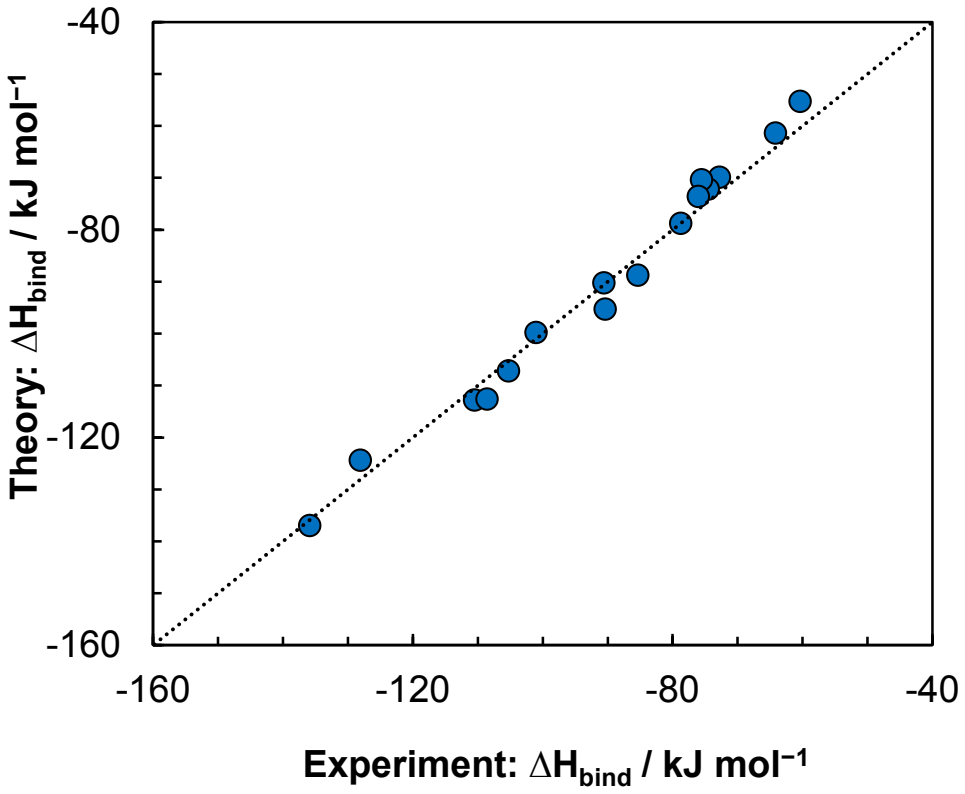


Fig. S3 Agreement between solution-phase theoretically predicted and experimentally determined binding enthalpies (ΔH_{bind})[a] for various monodentate [BF_3(Ligand)] complexes. The dashed line indicates perfect agreement between the theoretically computed and experimentally determined values.

3.2 Addition rate coefficients

To further confirm the accuracy of the theoretical methodology used in this study for kinetics, we benchmarked theoretically predicted addition rate coefficients (k_{add}) against experimentally derived values for reactions involving similar radicals and ester substituted alkene species (see **Table S3**). Chemical structures of the abbreviated radicals and alkenes listed in **Table S3** are provided in section 7. Experimental values were taken from references 19-22. We note excellent quantitative agreement (to within a factor of 3) between the theoretically predicted and experimentally derived k_{add} values. Moreover, theoretical methodology accurately predicts the effects of remote radical and alkene substituents on reactivity. For instance, theory correctly predicts that the T rad is more reactive towards n-butyl acrylate (nBA) than the B rad. The reduced reactivity of the M rad towards tert-butyl acrylate (tBA) and tert-butyl methacrylate (tBMA) as compared with nBA is also correctly predicted by this theoretical methodology.

Table S3 Theoretically predicted and experimentally derived addition rate coefficients (k_{add}) for similar radical reactions to those examined in this study (see section 5.2).

Radical	Alkene	Theory[a]		Experiment[a]	
		$\Delta G^{\ddagger}$(sol)	k_{add}(sol)	k_{add}(sol)	Ref
Cumyl	MMA	55.5	2.0×10^3	2.7×10^3	19
Benzyl	MMA	54.6	2.8×10^3	2.1×10^3	19
B rad	nBA	46.2	9.9×10^4	2.7×10^5	20
T rad	nBA	43.5	3.0×10^5	5.5×10^5	20
M rad	nBA	33.8	1.5×10^7	2.9×10^7	21
M rad	tBA	36.1[b]	6.0×10^6	1.5×10^7	22
M rad	tBMA	39.4	1.6×10^6	3.0×10^6	22

[a] $\Delta G^{\ddagger}$ values are given in kJ mol^{-1} and k_{add}(sol) values in L mol^{-1} s^{-1}. [b] The effective barrier, as two near transition state conformations were identified.

The close correlation between the theoretically predicted and experimentally derived k_{add} values is illustrated graphically in **Fig. S4**.

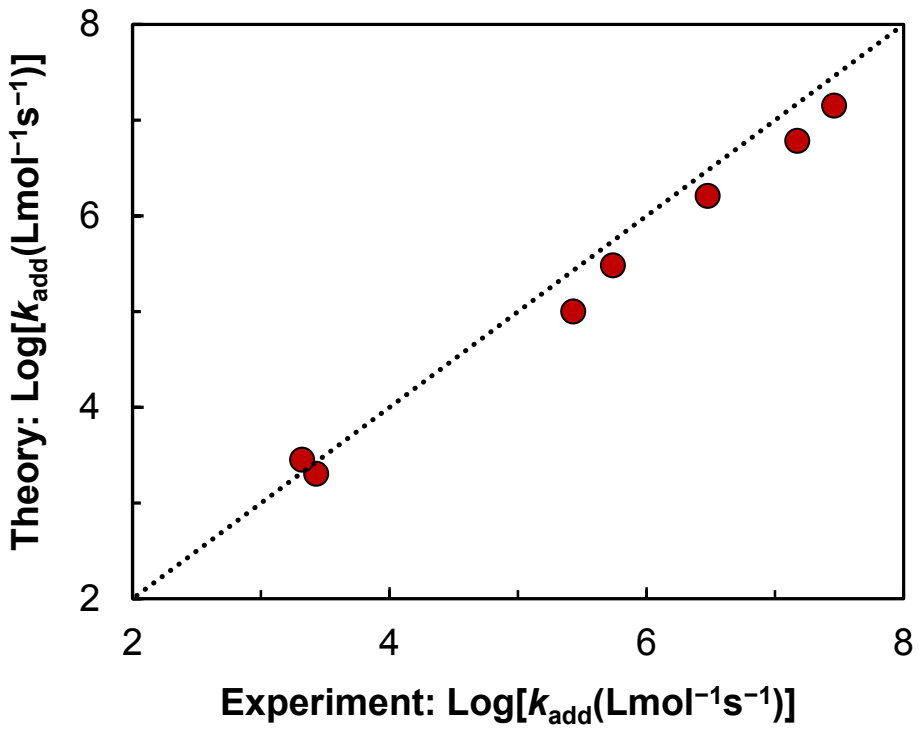


Fig. S4 Theoretically predicted and experimentally derived radical addition rate coefficients (k_{add}) for the species given in **Table S3**. The dashed diagonal line indicates perfect agreement between theoretical predictions and the corresponding experimental values.

4. Neutral $AlCl_3$ Complexes with MMMP and DMPA

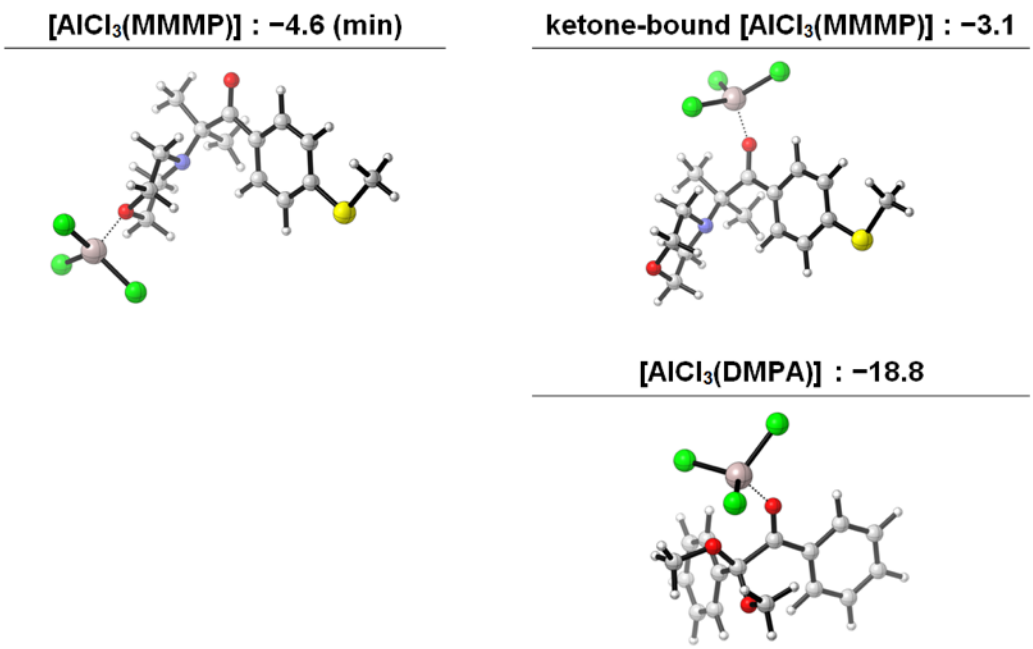


Fig. S5 Predicted coordination structures of neutral [$AlCl_3$(MMMP)] and [$AlCl_3$(DMPA)] complexes. The Gibbs Free Binding Energy of each photoinitiator complex, relative to competing solvation by MMA monomer, is indicated in kJ mol^{-1}.

5. Fragmentation pathways for MMMP and DMPA on their triplet surfaces.

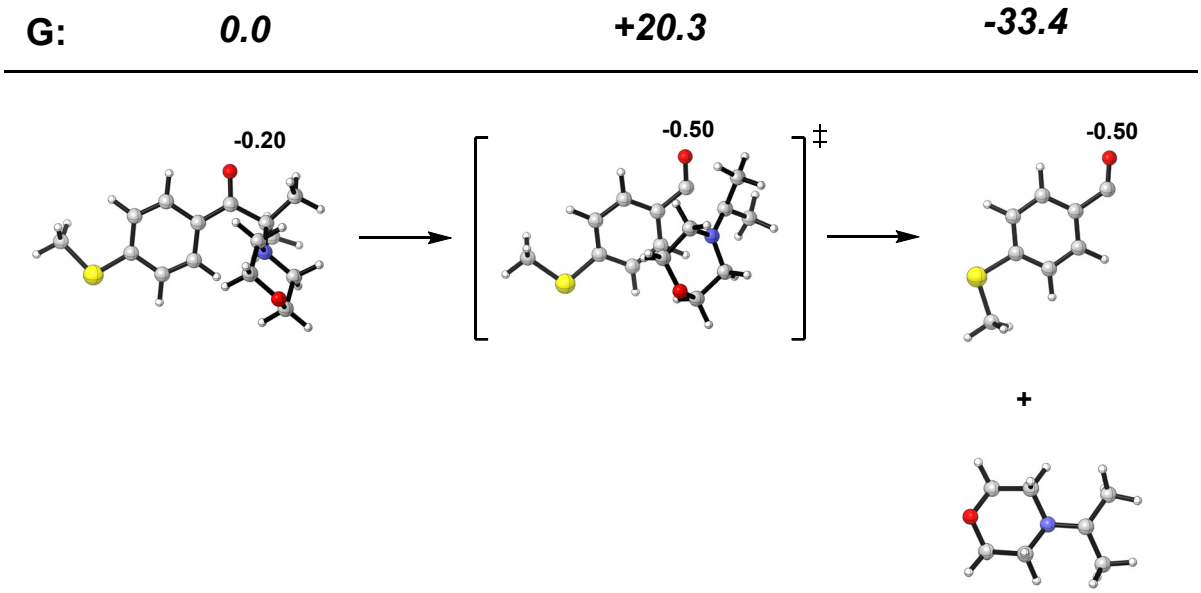


Fig. S6 The (semi-quantitative) free-energy for fragmentation of triplet MMMP (in kJ mol^{-1}), calculated at the UM06-2X/6-31+G(d,p) level of theory. Natural atomic charges (from a Natural Bond Order analysis) for the ketone oxygen atom for each species are also given. Note that the natural atomic charge is given for MMMP's T_2 ($n\pi^*$) state but the energy for fragmentation is given relative to MMMP's optimized T_1 ($\pi\pi^*$) state.

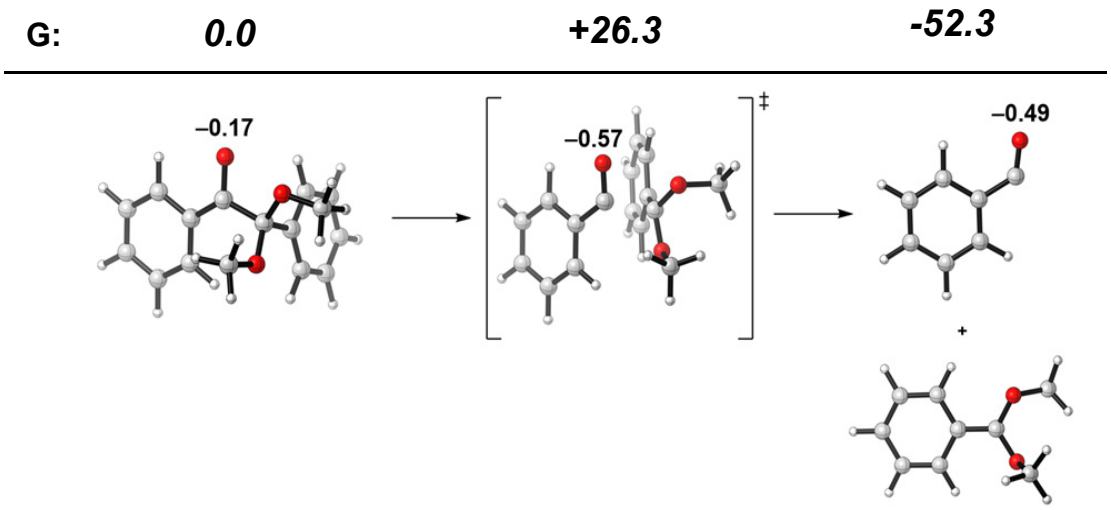


Fig. S7 The fragmentation of triplet DMPA, with relative free-energies (given in kJ mol^{-1}) calculated at the UM06-2X/6-31+G(d,p) level of theory. Natural atomic charges (from a Natural Bond Order analysis) for the ketone oxygen atom for each species are also given.

6. TD-DFT Calculations

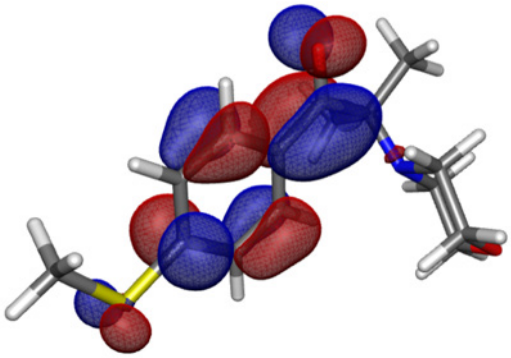
6.1 Raw TD-DFT data and principal molecular orbitals

Tables S4 – S11 contain raw TD-DFT results, with the principal molecular orbitals of interest illustrated in Fig S7 – S14. For brevity, transitions with coefficients of < 0.2 were omitted.

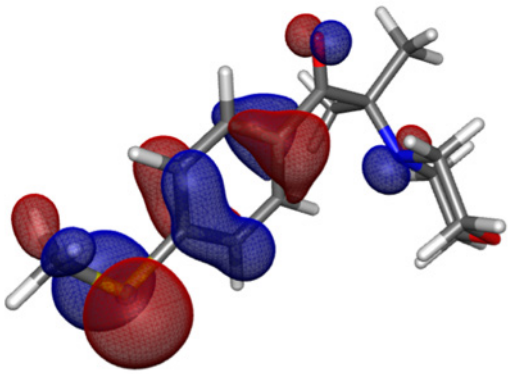
Table S4 TD-DFT excitation energies, oscillator strengths and dominant transitions with their respective contributions for MMMP.

Excited State	Oscillator Strength	Vertical Excitation Energy (eV)	Excitation Character[a]	
			Transition	Coefficient
S_1	0.0003	3.7205	71 → 76	-0.28490
			72 → 76	0.44157
			74 → 76	-0.29643
S_2	0.4632	4.3955	75 → 76	0.66154
S_3	0.1270	4.5835	75 → 76	0.60547
T_1	0.0000	3.3199	70 → 76	0.21576
			75 → 76	0.62244
T_2	0.0000	3.3599	71 → 76	-0.28687
			72 → 76	0.43306
			74 → 76	-0.26233
T_3	0.0000	4.4116	73 → 76	0.38897
			74 → 76	0.52017

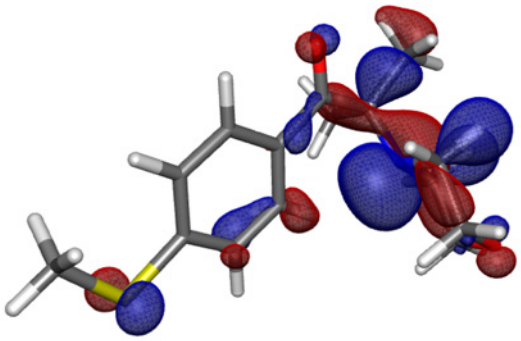
Fig. S8 UM06-2X/6-31+G(d,p) Molecular Orbitals for MMMP



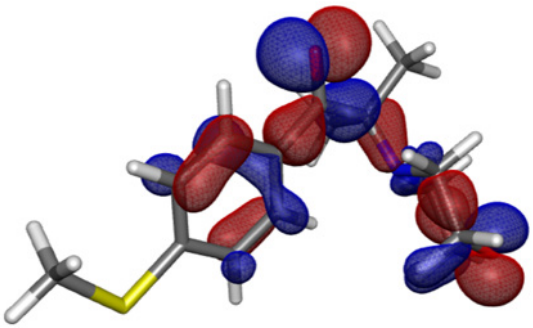
Orbital 76 (LUMO)



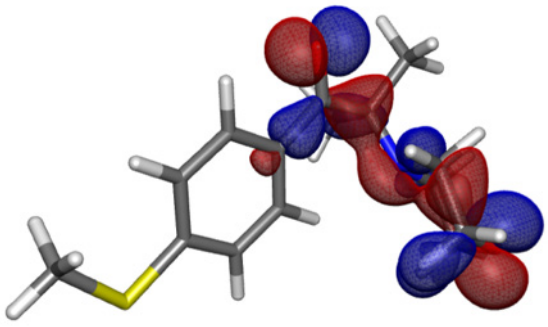
Orbital 75 (HOMO)



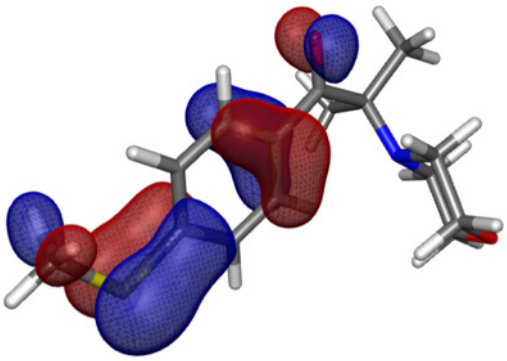
Orbital 74



Orbital 72



Orbital 71

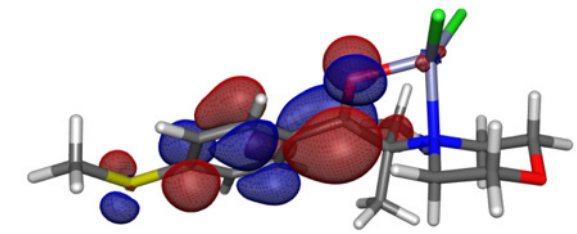


Orbital 70

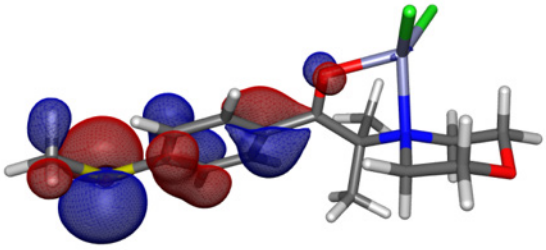
Table S5 TD-DFT excitation energies, oscillator strengths and dominant transitions with their respective contributions for [$ZnCl_2$(MMMP)]

Excited State	Oscillator Strength	Vertical Excitation Energy (eV)	Excitation Character[a]	
			Transition	Coefficient
S_1	0.6485	4.0164	107 → 108	0.67591
S_2	0.0333	4.3651	97 → 108	0.48321
			102 → 108	0.21661
S_3	0.0039	4.7694	104 → 108	0.52917
			107 → 109	-0.40148
T_1	0.0000	3.0631	107 → 108	0.65045
T_2	0.0000	4.0087	97 → 108	0.47197
			102 → 108	0.20033
T_3	0.0000	4.3310	104 → 108	0.65521
T_4	0.0000	4.5285	107 → 109	0.60368
			107 → 110	-0.216090

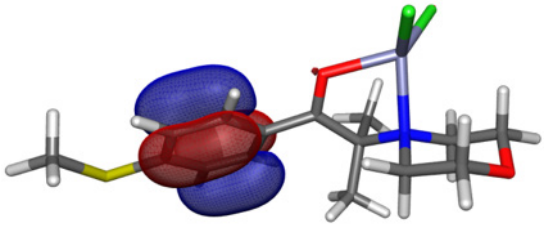
Fig. S9 UM06-2X/6-31+G(d,p) Molecular Orbitals for [$ZnCl_2$(MMMP)]



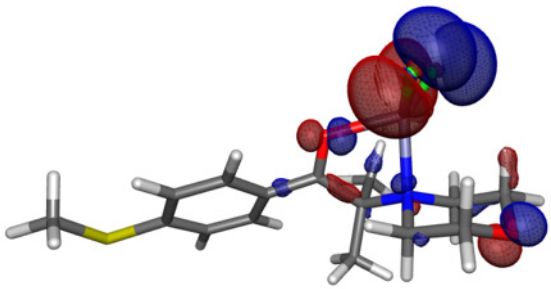
Orbital 108 (LUMO)



Orbital 107 (HOMO)



Orbital 104



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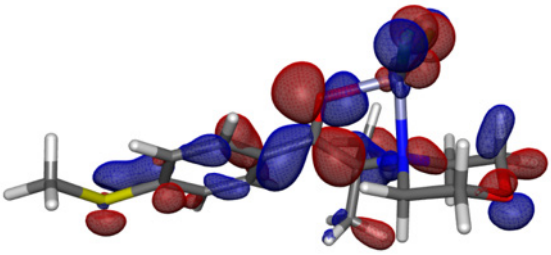
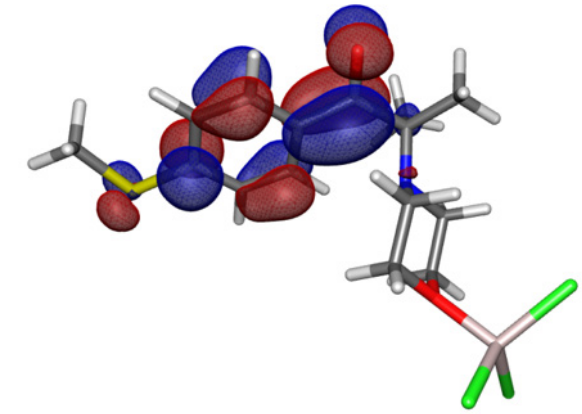


Orbital 97

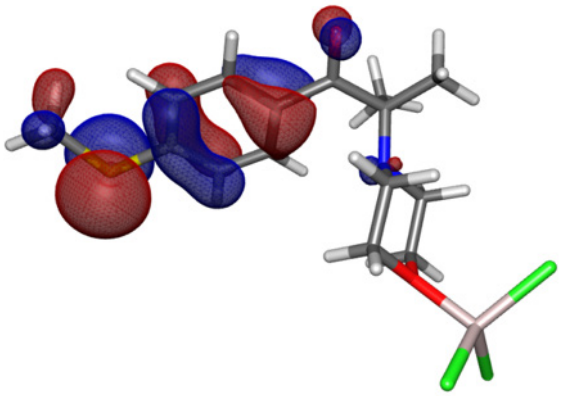
Table S6 TD-DFT excitation energies, oscillator strengths and dominant transitions with their respective contributions for [$AlCl_3$(MMMP)].

Excited State	Oscillator Strength	Vertical Excitation Energy (eV)	Excitation Character[a]	
			Transition	Coefficient
S_1	0.0014	3.7346	104 → 108	0.51841
			106 → 108	-0.30871
S_2	0.5746	4.3941	107 → 108	0.68601
S_3	0.0190	4.7827	105 → 108	0.31045
			106 → 108	0.52749
			107 → 110	-0.22084
T_1	0.0000	3.2736	103 → 108	-0.20114
			104 → 108	0.23513
			107 → 108	0.58078
T_2	0.0000	3.3888	104 → 108	0.47343
			106 → 108	-0.25193
			107 → 108	-0.28322
T_3	0.0000	4.4653	105 → 108	0.53734
			106 → 108	0.29927
			107 → 110	0.22710

Fig. S10 UM06-2X/6-31+G(d,p) Molecular Orbitals for [$AlCl_3$(MMMP)]



Orbital 108 (LUMO)



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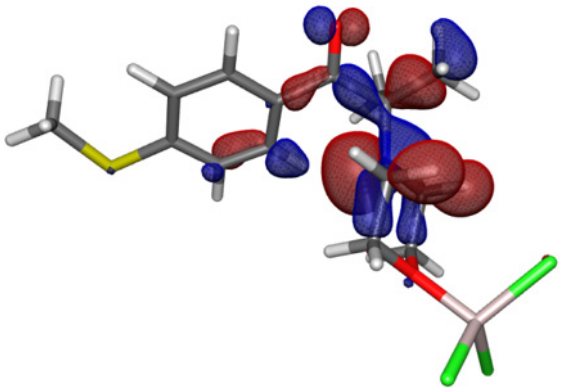

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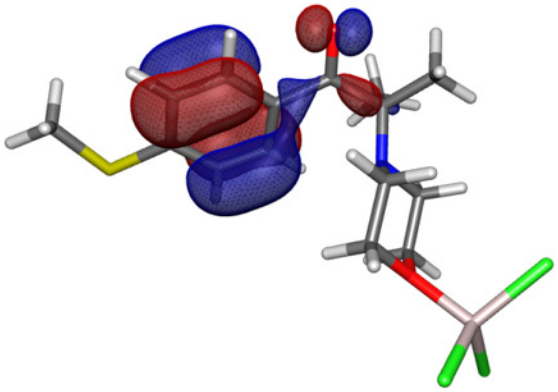

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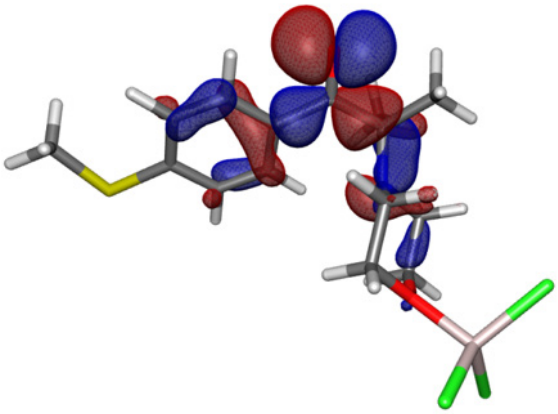

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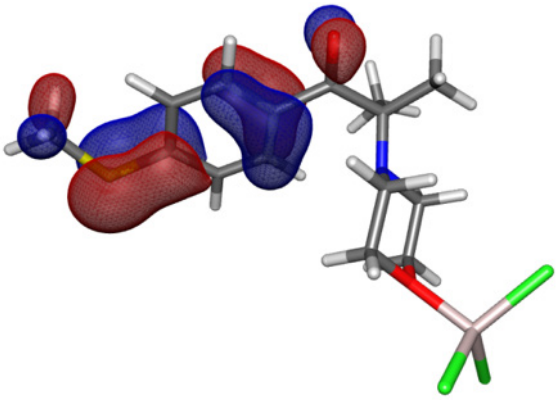
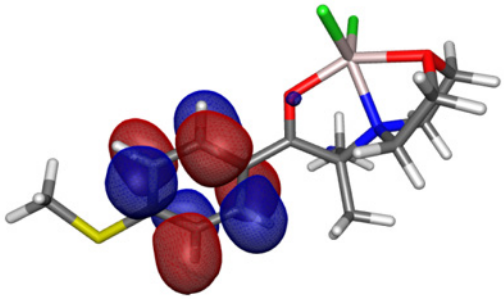


Orbital 103

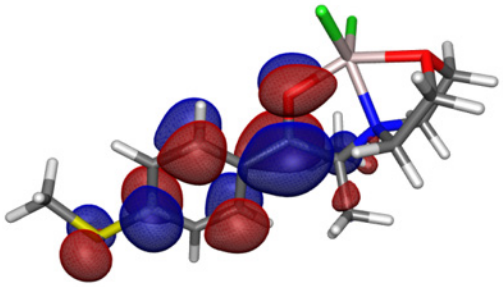
Table S7 TD-DFT excitation energies, oscillator strengths and dominant transitions with their respective contributions for $[AlCl_2(MMMP)]^+$.

Excited State	Oscillator Strength	Vertical Excitation Energy (eV)	Excitation Character[a]	
			Transition	Coefficient
S_1	0.8278	3.5831	98 → 99	0.69395
S_2	0.0250	4.4194	97 → 99	0.66560
S_3	0.0025	4.8513	89 → 99	0.41165
			90 → 99	−0.39042
T_1	0.0000	2.4888	98 → 99	0.67393
T_2	0.0000	3.7628	97 → 99	0.69029
T_3	0.0000	4.5418	94 → 99	−0.29472
			96 → 99	0.29588
			97 → 100	−0.36702
			98 → 100	−0.22276
T_4	0.0000	4.5594	89 → 99	0.40356
			90 → 99	−0.36905

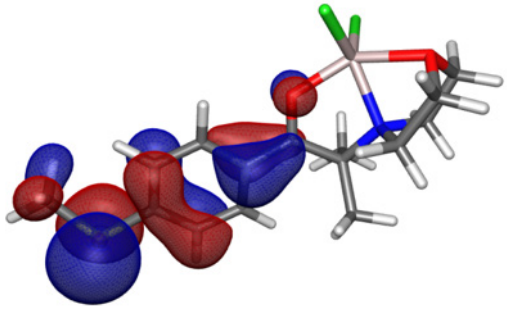
Fig. S11 UM06-2X/6-31+G(d,p) Molecular Orbitals for $[AlCl_2(MMMP)]^+$



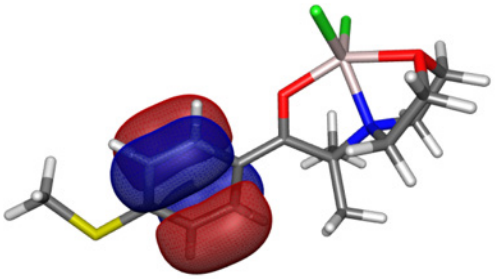
Orbital 100



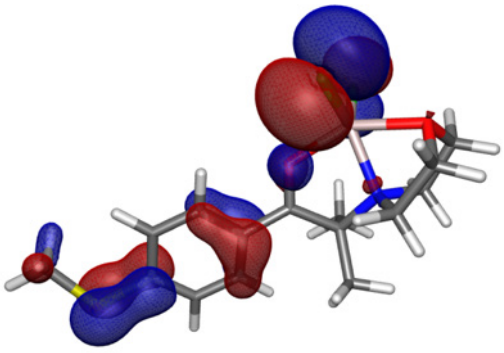
Orbital 99 (LUMO)



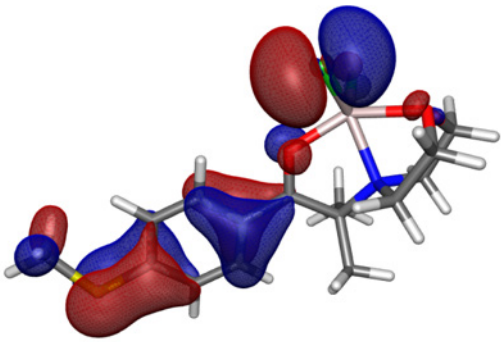
Orbital 98 (HOMO)



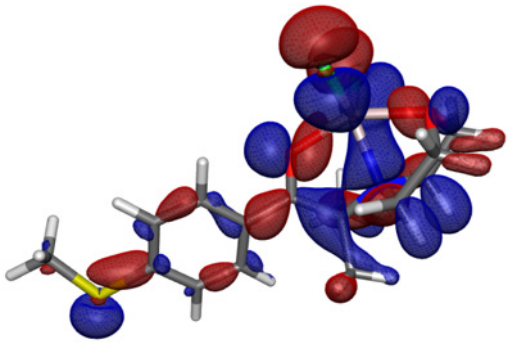
Orbital 97



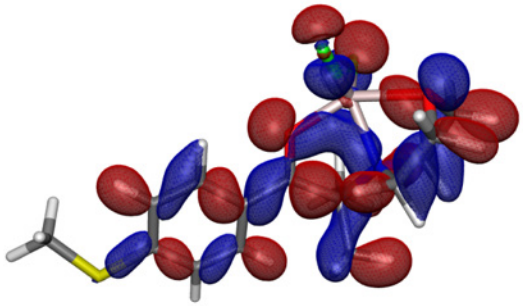
Orbital 96



Orbital 94



Orbital 90

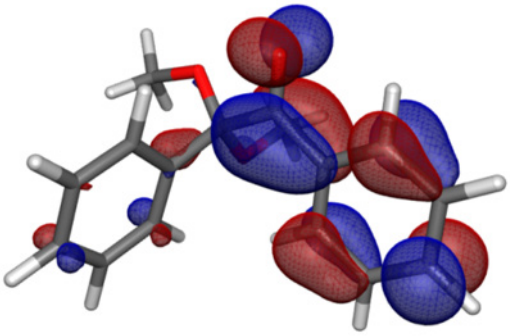


Orbital 89

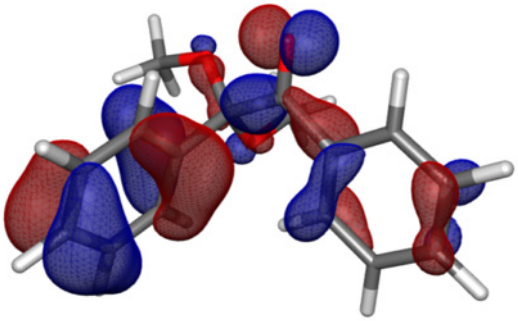
Table S8 TD-DFT excitation energies, oscillator strengths and dominant transitions with their respective contributions for DMPA.

Excited State	Oscillator Strength	Vertical Excitation Energy (eV)	Excitation Character[a]	
			Transition	Coefficient
S_1	0.0044	3.5908	64 → 69	0.37864
			65 → 69	-0.30360
			68 → 69	0.37464
S_2	0.0229	4.9711	65 → 69	-0.35393
			66 → 69	0.40402
			67 → 69	0.26905
			68 → 69	-0.21544
S_3	0.3310	5.1844	65 → 69	0.35113
			66 → 69	0.42380
			68 → 69	0.37727
T_1	0.0000	3.1990	64 → 69	0.36018
			65 → 69	-0.31690
			68 → 69	0.35401
T_2	0.0000	3.7557	65 → 69	0.36080
			66 → 69	0.46176
			68 → 69	0.20609
T_3	0.0000	4.2566	68 → 69	0.21904
			69 → 70	0.33885

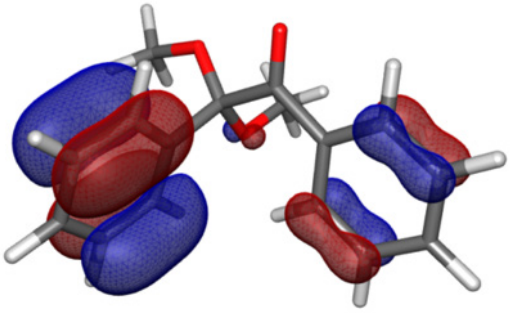
Fig. S12 UM06-2X/6-31+G(d,p) Molecular Orbitals for DMPA



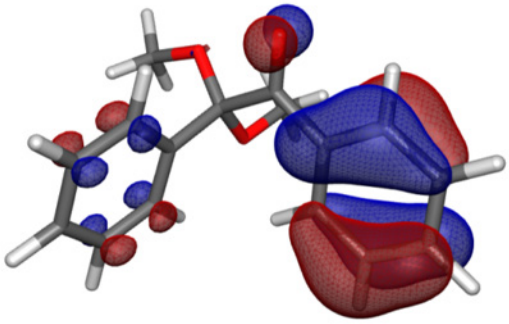
Orbital 69 (LUMO)



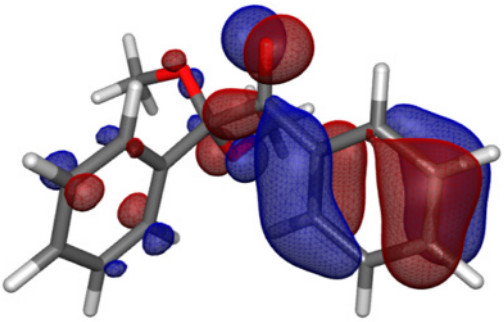
Orbital 68 (HOMO)



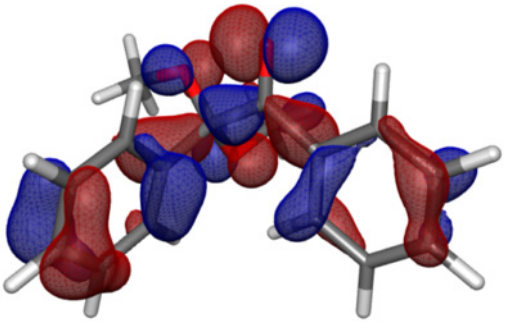
Orbital 67



Orbital 66



Orbital 65

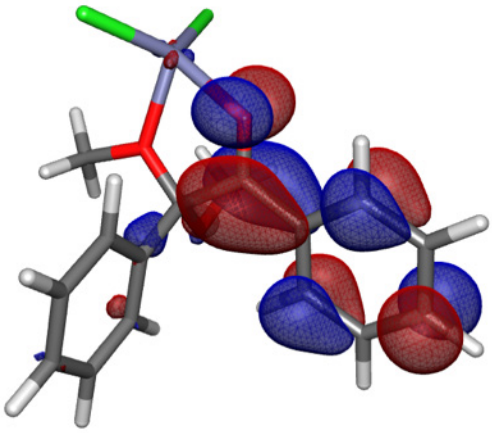


Orbital 64

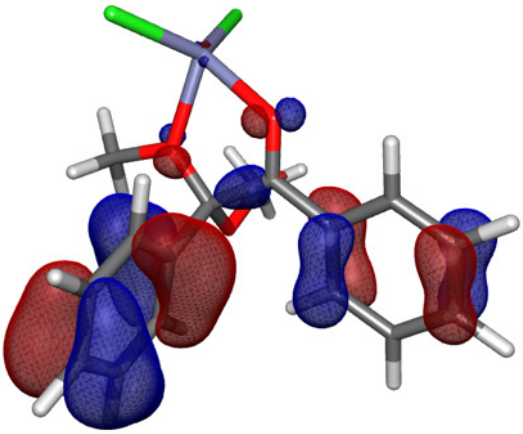
Table S9 TD-DFT excitation energies, oscillator strengths and dominant transitions with their respective contributions for [$ZnCl_2$(DMPA)].

Excited State	Oscillator Strength	Vertical Excitation Energy (eV)	Excitation Character[a]	
			Transition	Coefficient
S_1	0.0241	4.0125	92 → 101	0.40707
			100 → 101	-0.36683
S_2	0.0261	4.4730	98 → 101	0.55826
			99 → 101	0.21492
			100 → 101	0.29582
S_3	0.3652	4.6508	97 → 101	0.38518
			98 → 101	-0.29068
			100 → 101	0.41178
T_1	0.0000	3.3804	97 → 101	0.51726
			98 → 101	-0.27207
			100 → 101	0.30392
T_2	0.0000	3.7181	92 → 101	0.39812
			97 → 101	0.23475
			100 → 101	-0.28349
T_3	0.0000	3.7791	97 → 101	0.20548
			98 → 101	0.58301
			100 → 101	0.21450
T_4	0.0000	4.2341	99 → 105	-0.25129
			100 → 102	0.37985

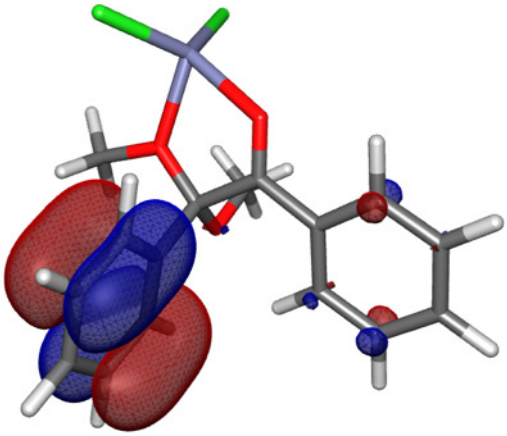
Fig. S13 UM06-2X/6-31+G(d,p) Molecular Orbitals for [$ZnCl_2$(DMPA)].



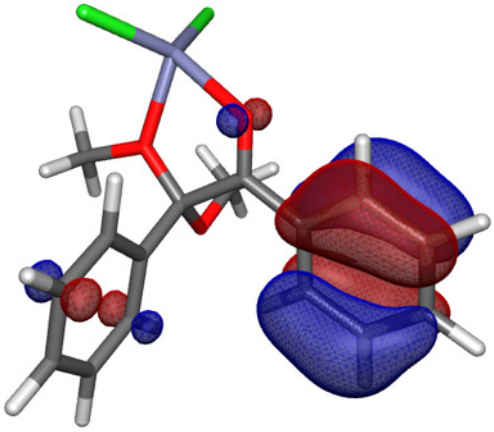
Orbital 101 (LUMO)



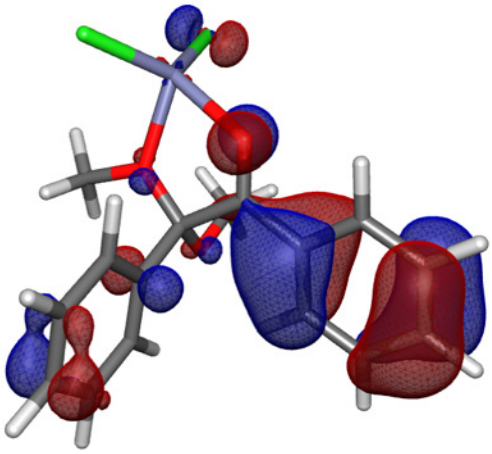
Orbital 100 (HOMO)



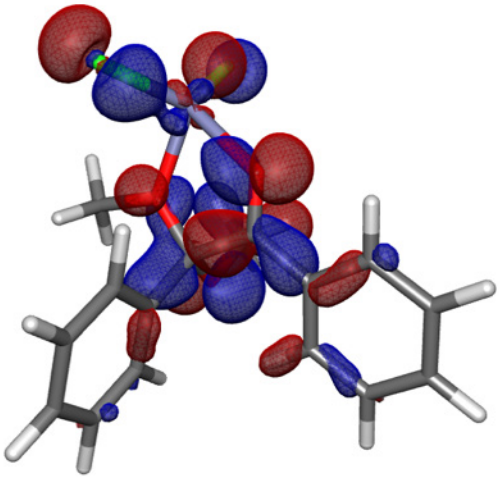
Orbital 99



Orbital 98



Orbital 97

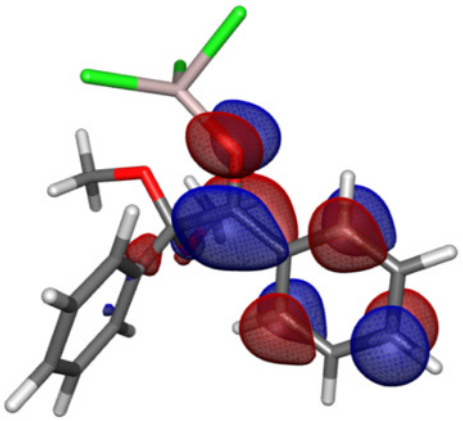


Orbital 92

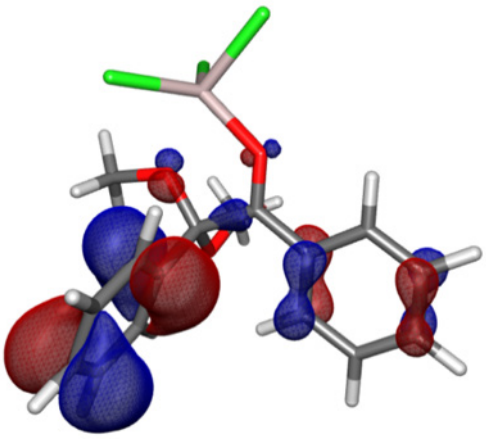
Table S10 TD-DFT excitation energies, oscillator strengths and dominant transitions with their respective contributions for [$AlCl_3$(DMPA)].

Excited State	Oscillator Strength	Vertical Excitation Energy (eV)	Excitation Character[a]	
			Transition	Coefficient
S_1	0.0710	4.0130	90 → 101	-0.25418
			100 → 101	0.56907
S_2	0.0453	4.1769	97 → 101	0.64562
S_3	0.2666	4.4164	90 → 101	0.29100
			95 → 101	0.38829
			100 → 101	0.30938
T_1	0.0000	3.1265	95 → 101	0.58710
			100 → 101	0.27088
T_2	0.0000	3.4331	97 → 101	0.62844
			100 → 101	0.20850
T_3	0.0000	3.8344	90 → 101	-0.33326
			95 → 101	-0.22911
			100 → 101	0.36151
T_4	0.0000	4.2021	99 → 101	0.34055
			99 → 104	0.35094
			100 → 102	-0.34059

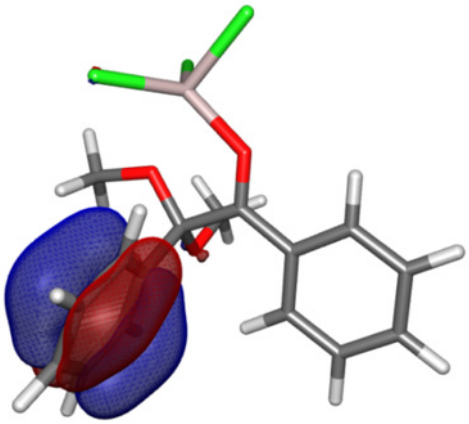
Fig. S14 UM06-2X/6-31+G(d,p) Molecular Orbitals for [$AlCl_3$(DMPA)].



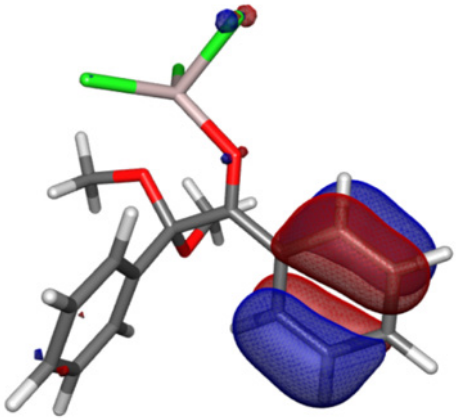
Orbital 101 (LUMO)



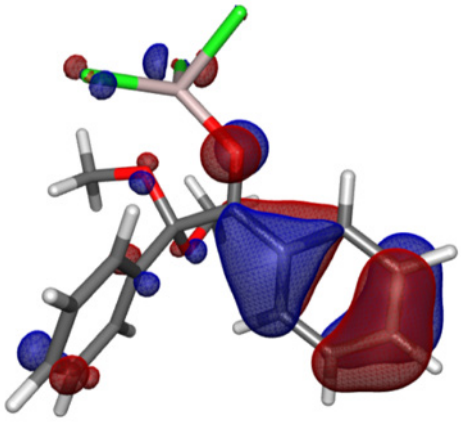
Orbital 100



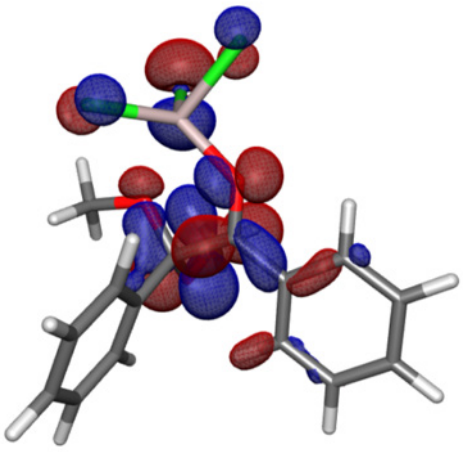
Orbital 99



Orbital 97



Orbital 95

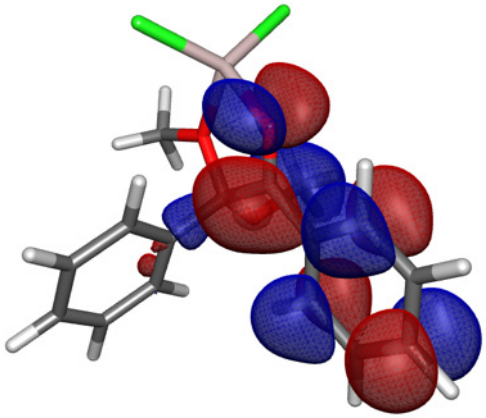


Orbital 90

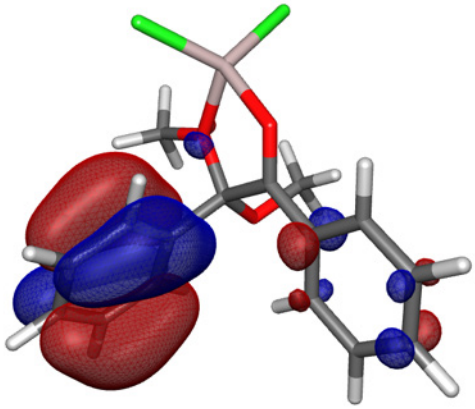
Table S11 TD-DFT excitation energies, oscillator strengths and dominant transitions with their respective contributions for $[AlCl_2(DMPA)]^+$.

Excited State	Oscillator Strength	Vertical Excitation Energy (eV)	Excitation Character[a]	
			Transition	Coefficient
S_1	0.0469	3.8027	89 → 92	−0.40868
			90 → 92	0.46812
			91 → 92	−0.29575
S_2	0.1778	3.9127	89 → 92	0.54327
			90 → 92	0.20620
			91 → 92	−0.34863
S_3	0.0053	4.1410	90 → 92	0.44949
			91 → 92	0.51767
S_4	0.3874	4.4205	86 → 92	0.25314
			88 → 92	0.61232
T_1	0.0000	3.0712	89 → 92	0.64826
			90 → 92	−0.21939
T_2	0.0000	3.8358	86 → 92	0.21377
			88 → 92	0.28073
			90 → 92	0.43500
			91 → 92	−0.27433
T_3	0.0000	4.0234	90 → 92	0.33084
			91 → 92	0.55164
T_4	0.0000	4.2920	86 → 92	0.25926
			90 → 93	−0.27673
			91 → 93	0.33458
			91 → 96	0.22241

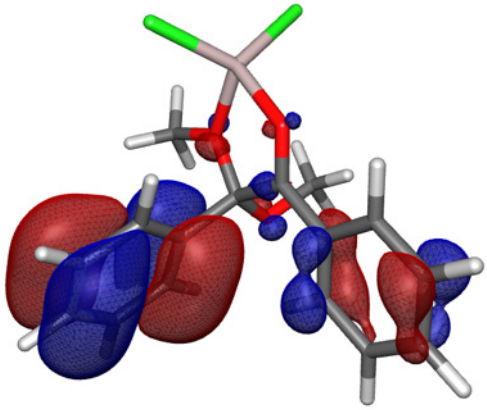
Fig. S15 UM06-2X/6-31+G(d,p) Molecular Orbitals for $[AlCl_2(DMPA)]^+$.



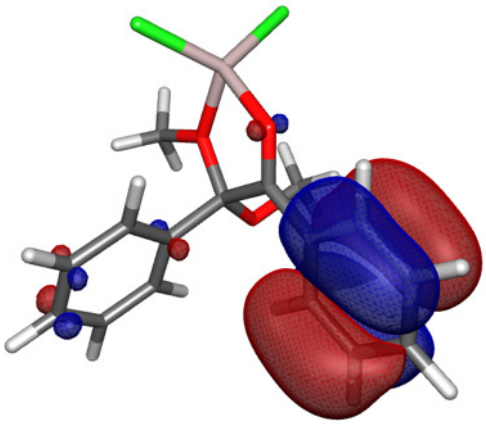
Orbital 92 (LUMO)



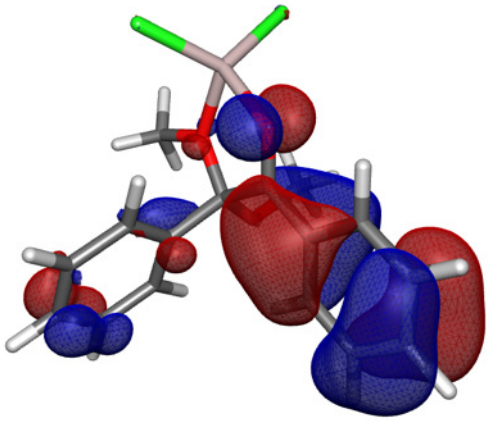
Orbital 91



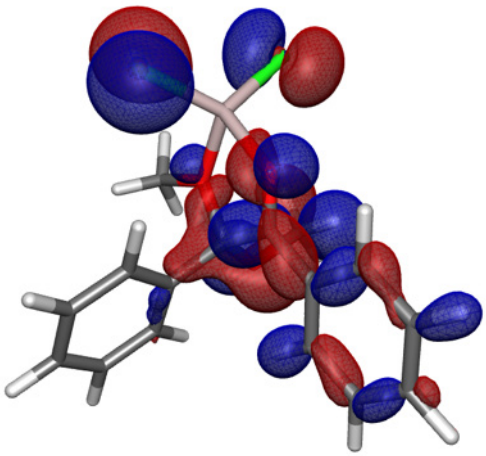
Orbital 90



Orbital 89



Orbital 88

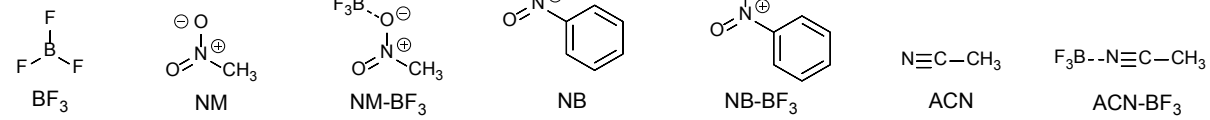


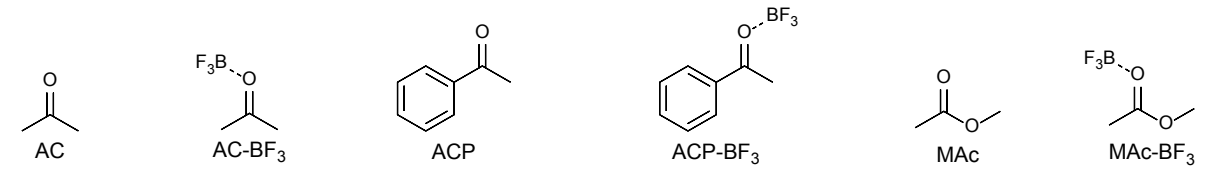
Orbital 86

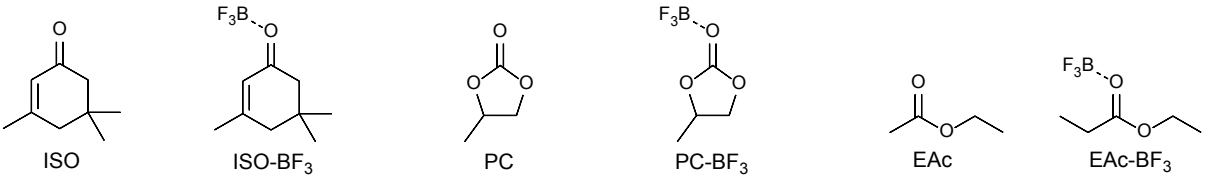
7. Chemical structures and their Abbreviations

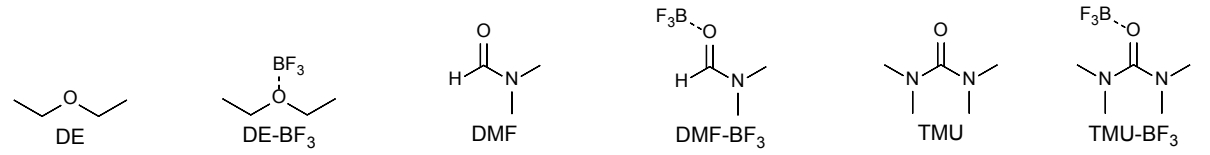
Chemical structures of all the species examined in this work and their abbreviations.

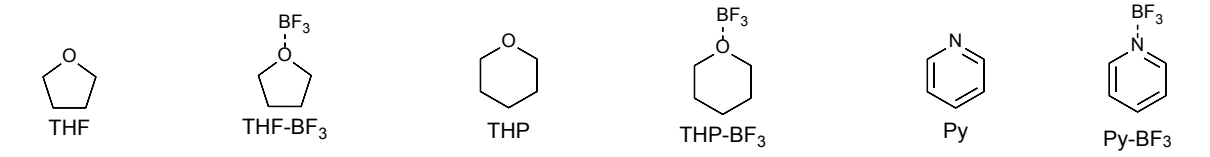
7.1 Benchmarking: BF_3 binding enthalpies

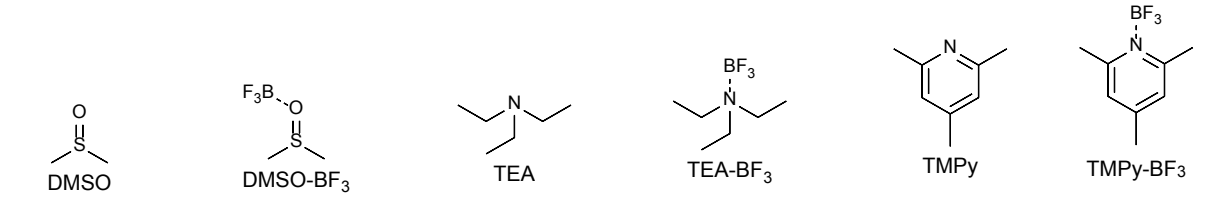




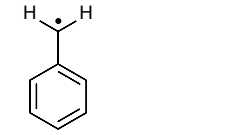


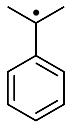


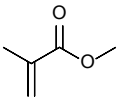




7.2 Benchmarking: Addition rate coefficients


Benzyl rad


Cumyl rad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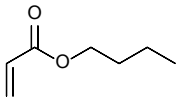
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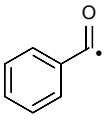
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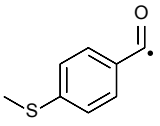
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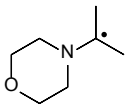
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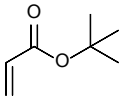
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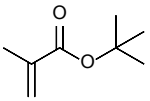
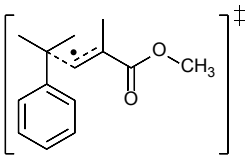
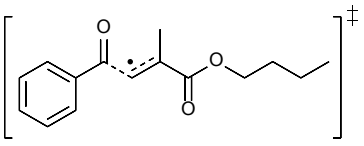
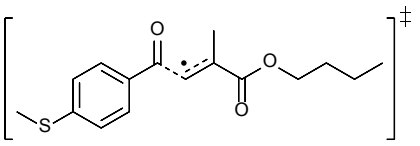
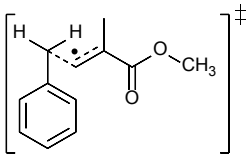
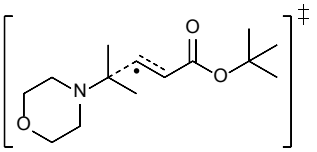

tBMA

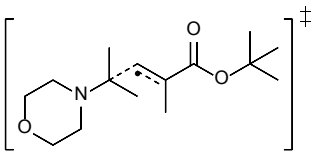

Cumyl rad-MMA TS

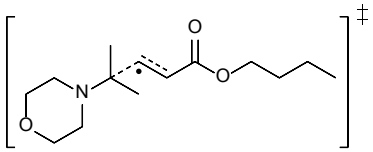

B rad-nBA TS


T rad-nBA TS

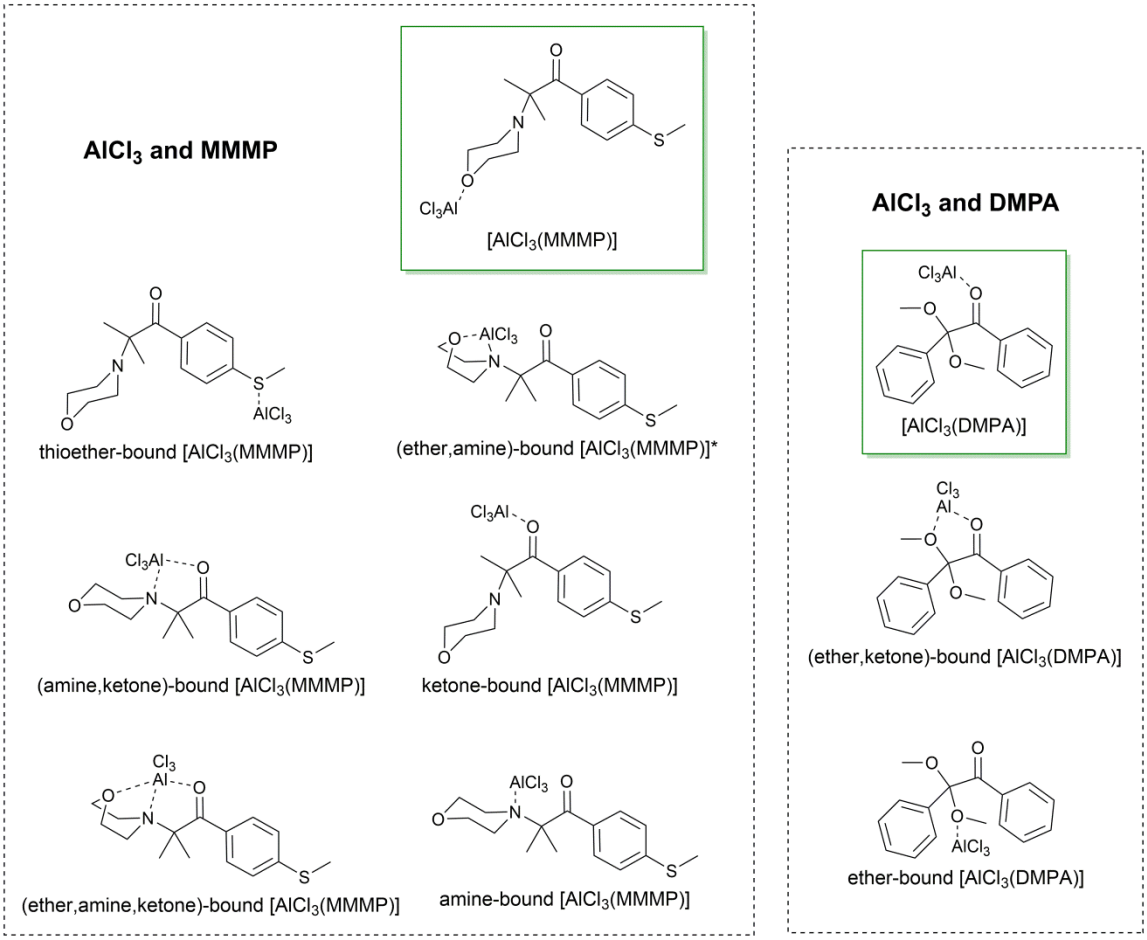

Benzyl rad-MMA TS

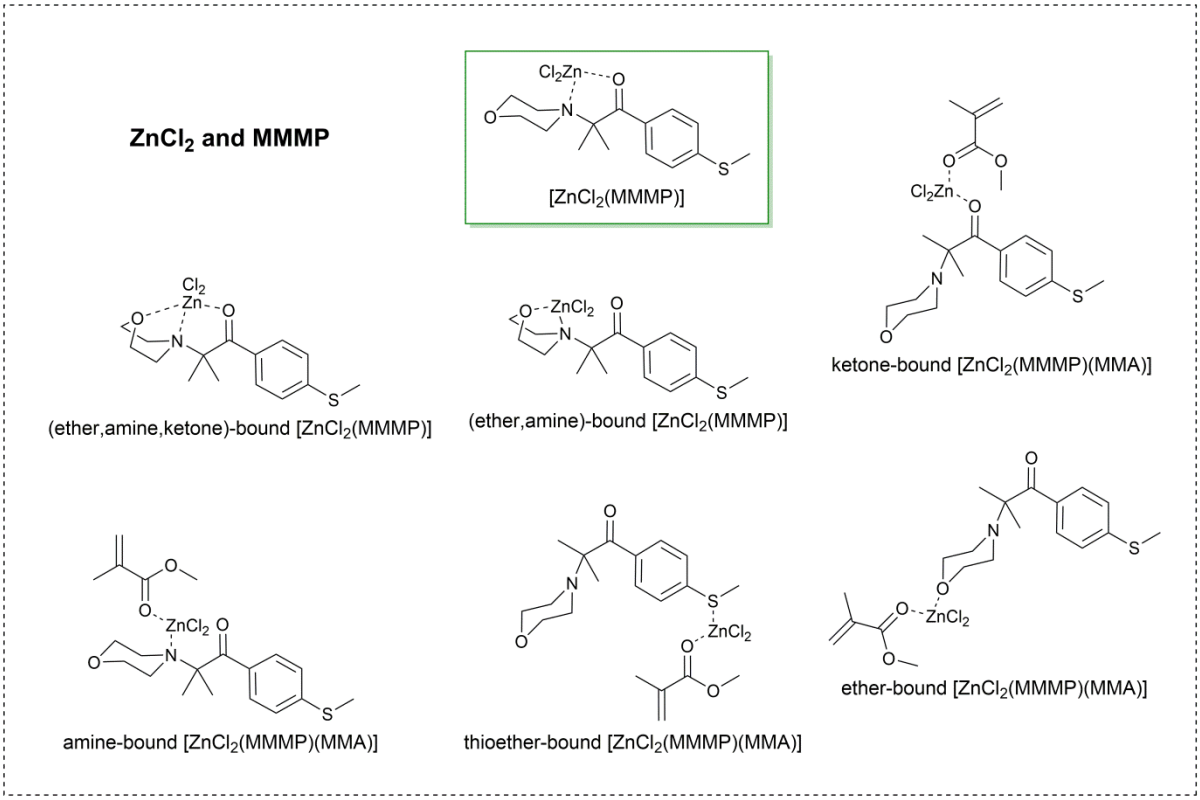

M rad-tBA TS


M rad-tBMA TS


M rad-nBA TS

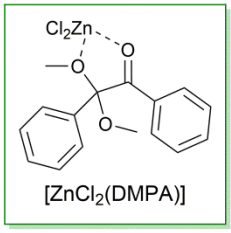
7.3 Lewis acid binding modes to MMMP and DMPA



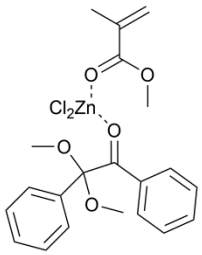


*Indicates complex was not stable

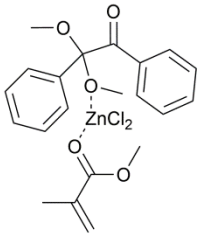
$ZnCl_2$ and DMPA



[$ZnCl_2$(DMPA)]

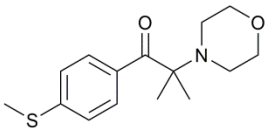


ketone-bound [$ZnCl_2$(DMPA)(MMA)]

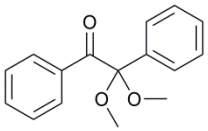


ether-bound [$ZnCl_2$(DMPA)(MMA)]

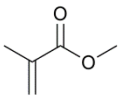
Miscellaneous



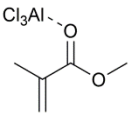
MMMP



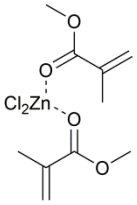
DMPA



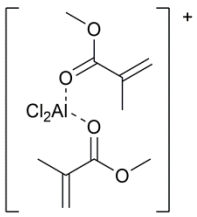
MMA



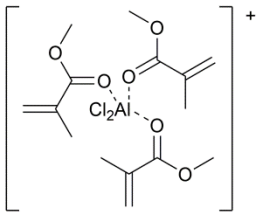
$AlCl_3$(MMA)



$ZnCl_2$(MMA)2

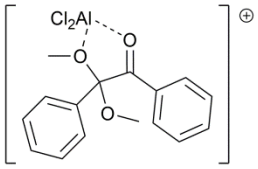


$AlCl_2(MMA)_2^+$

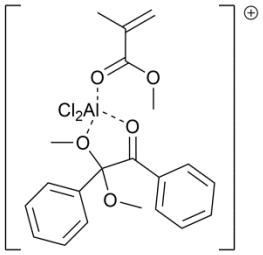


$AlCl_2(MMA)_3^+$

$AlCl_2^+$ and DMPA

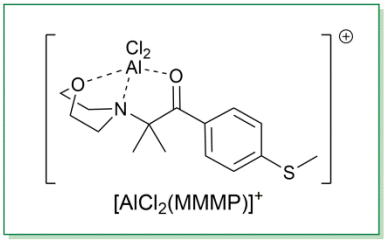


$[AlCl_2(DMPA)]^+$

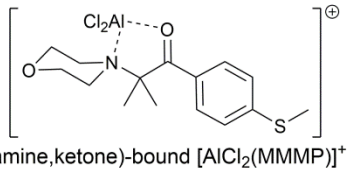


$[AlCl_2(DMPA)(MMA)]^+$

$AlCl_2^+$ and MMMP

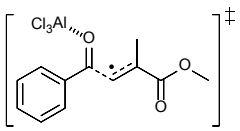


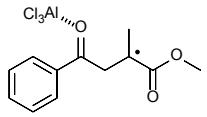
$[AlCl_2(MMMP)]^+$

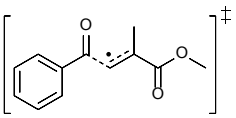


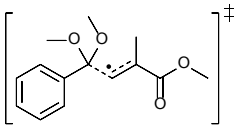
(amine,ketone)-bound $[AlCl_2(MMMP)]^+$

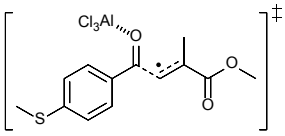
7.4 RSE and Rate Coefficient Section

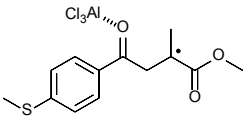

B rad/$AlCl_3$-MMA TS

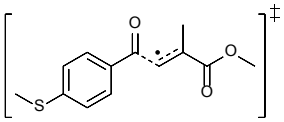

B rad/$AlCl_3$-MMA

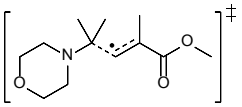

B rad-MMA TS

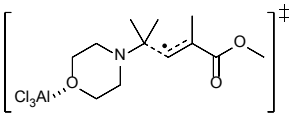

D rad-MMA TS

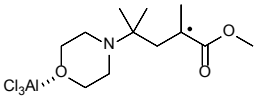

T rad/$AlCl_3$-MMA TS

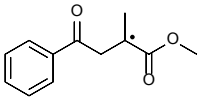

T rad/$AlCl_3$-MMA

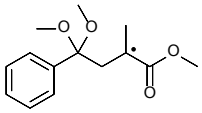

T rad-MMA TS

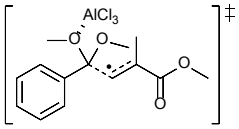

M rad-MMA TS

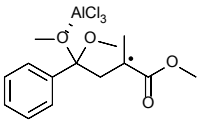

Obound M rad/$AlCl_3$-MMA TS

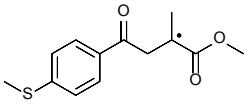

Obound M rad/$AlCl_3$-MMA

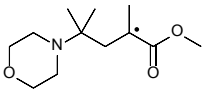

B rad-MMA

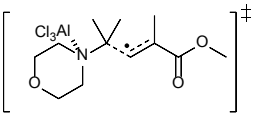

D rad-MMA

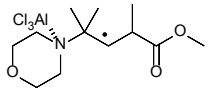

D rad/$AlCl_3$-MMA TS

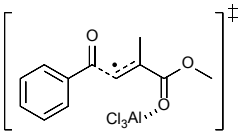

D rad/$AlCl_3$-MMA

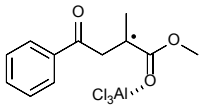

T rad-MMA

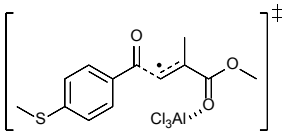

M rad-MMA

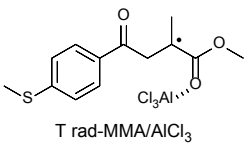

Nbound M rad/$AlCl_3$-MMA TS

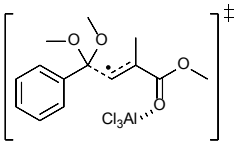

Nbound M rad/$AlCl_3$-MMA

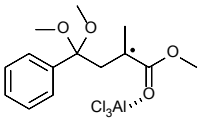

B rad-MMA/$AlCl_3$ TS

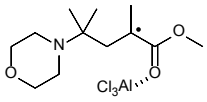

B rad-MMA/$AlCl_3$ TS

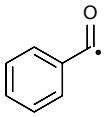

T rad-MMA/$AlCl_3$ TS


T rad-MMA/$AlCl_3$

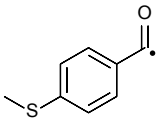

D rad-MMA TS


D rad-MMA

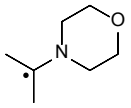

M rad-MMA/$AlCl_3$



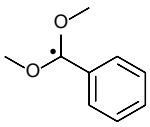
B rad



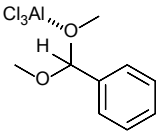
T rad



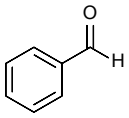
M rad



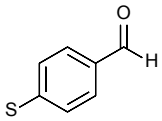
D rad



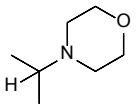
D rad-H $AlCl_3$



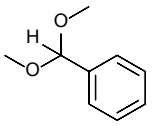
B rad-H



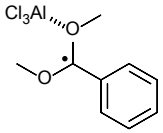
T rad-H



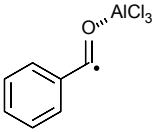
M rad-H



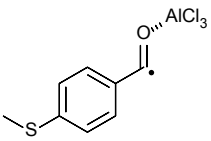
D rad-H



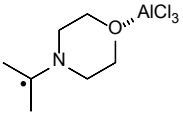
D rad $AlCl_3$



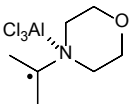
B rad $AlCl_3$



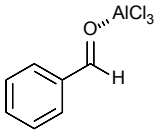
T rad $AlCl_3$



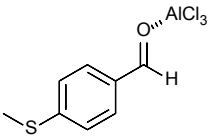
M rad $_{(O)}$ $AlCl_3$



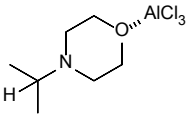
M rad $_{(N)}$ $AlCl_3$



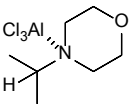
B rad-H $AlCl_3$



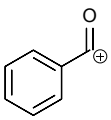
T rad-H $AlCl_3$



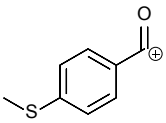
M rad-H $_{(O)}$ $AlCl_3$



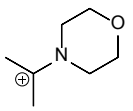
M rad-H $_{(N)}$ $AlCl_3$



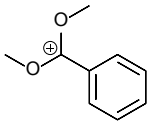
B cation



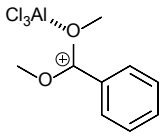
T cation



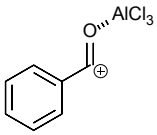
M cation



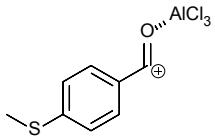
D cation



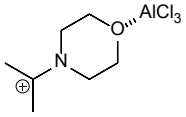
D cation $AlCl_3$



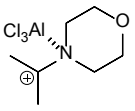
B cation $AlCl_3$



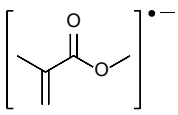
T cation $AlCl_3$



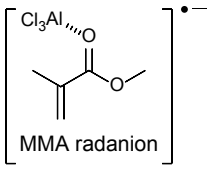
M cation $_{(O)}$ $AlCl_3$



M cation $_{(N)}$ $AlCl_3$



MMA radanion



MMA radanion

8. Raw Energies

Contributions of raw energies, thermal corrections, entropies and solvation corrections to the total Gibbs free-energies and enthalpies. Note that the standard state gas to solution-phase correction has been included in the solvation energies (G_{solv}). Unless otherwise specified, units are given in hartrees.

8.1 Benchmarking: BF_3 binding enthalpies

Table S12. Raw energies for BF_3 complexation reactions.

Species	Thermal Corrections (25 °C)			Raw Energies					Thermochemistry (25 °C)	
	S (J/mol K)	Thermal correction	ZPVE	M06-2X/ 6-31+G(d,p)	RMP2/ 6-31G(d)	RMP2/ GTMP2Large	URCCSD(T)/ 6-31G(d)	G3(MP2)-RAD	G3(MP2)-RAD/ Enthalpy (Gas)	ΔG_{solv}
BF_3	255.04	0.004478	0.012108	-324.469850	-323.778485	-324.147578	-323.794642	-324.163735	-324.147149	-0.000921
NB	344.32	0.007818	0.100984	-436.586285	-435.466688	-435.926097	-435.548707	-436.008116	-435.899314	-0.010608
NB-BF_3	459.07	0.012475	0.114513	-761.070064	-759.256717	-760.081827	-759.355856	-760.180966	-760.053978	-0.021548
NM	290.43	0.005292	0.049113	-244.914447	-244.330157	-244.607955	-244.364206	-244.642004	-244.587599	-0.007503
NM-BF_3	376.60	0.008983	0.062614	-569.396965	-568.119777	-568.762519	-568.171058	-568.813800	-568.742203	-0.019071
ACN	242.75	0.004572	0.044325	-132.700778	-132.337032	-132.479991	-132.372451	-132.515410	-132.466513	-0.006964
ACN-BF_3	380.96	0.009045	0.058119	-457.186686	-456.127508	-456.640028	-456.178326	-456.690846	-456.623682	-0.022539
PC	330.42	0.007201	0.100790	-381.582412	-380.608465	-381.039433	-380.680242	-381.111210	-381.003219	-0.011933
PC-BF_3	437.14	0.011702	0.114766	-706.072593	-704.401755	-705.201206	-704.490799	-705.290250	-705.163782	-0.026446
MAc	325.68	0.007118	0.087841	-268.283531	-267.572691	-267.890086	-267.630948	-267.948343	-267.853384	-0.004852
MAc-BF_3	416.95	0.011042	0.102497	-592.781379	-591.373564	-592.058225	-591.449103	-592.133764	-592.020225	-0.016304
ACP	367.41	0.008873	0.134487	-384.744541	-383.661097	-384.079816	-383.762856	-384.181575	-384.038215	-0.012492
ACP-BF_3	461.57	0.013054	0.149056	-709.242553	-707.461458	-708.248071	-707.580563	-708.367176	-708.205066	-0.024834
EAc	355.82	0.008394	0.115424	-307.583443	-306.743358	-307.111976	-306.817760	-307.186378	-307.062560	-0.006643
EAc-BF_3	429.63	0.011648	0.129838	-632.080872	-630.542797	-631.279924	-630.634579	-631.371706	-631.230220	-0.018765
AC	301.41	0.006393	0.081610	-193.071904	-192.523480	-192.759206	-192.577732	-192.813458	-192.725455	-0.006893

AC-BF_3	392.78	0.010184	0.096361	-517.569919	-516.324546	-516.927338	-516.395919	-516.998711	-516.892166	-0.019901
DE	328.53	0.007813	0.133309	-233.556144	-232.845433	-233.154749	-232.923054	-233.232370	-233.091248	-0.004101
DE-BF_3	426.24	0.011745	0.148498	-558.057398	-556.652727	-557.327081	-556.746654	-557.421008	-557.260765	-0.016298
THP	308.35	0.006434	0.142853	-271.656363	-270.843982	-271.184244	-270.930041	-271.270303	-271.121016	-0.005629
THP-BF_3	403.25	0.010589	0.157891	-596.160962	-594.654939	-595.361062	-594.757106	-595.463229	-595.294749	-0.017421
THF	300.53	0.005894	0.114026	-232.352291	-231.670033	-231.958820	-231.739965	-232.028752	-231.908832	-0.005083
THF-BF_3	389.23	0.009747	0.129314	-556.858729	-555.482988	-556.136929	-555.569080	-556.223021	-556.083960	-0.017924
ISO	409.21	0.011498	0.205306	-426.442024	-425.172954	-425.682021	-425.308074	-425.817141	-425.600337	-0.012984
ISO-BF_3	501.25	0.015670	0.219740	-750.945731	-748.979317	-749.855785	-749.131617	-750.008085	-749.772675	-0.026704
TMPy	408.24	0.010694	0.166544	-366.091524	-365.000855	-365.418770	-365.114544	-365.532459	-365.355221	-0.010759
TMPy-BF_3	478.08	0.014079	0.182656	-690.601978	-688.816874	-689.600784	-688.947297	-689.731207	-689.534472	-0.021192
DMSO	307.49	0.006600	0.077558	-553.082805	-552.112111	-552.422164	-552.170704	-552.480757	-552.396599	-0.011711
DMSO-BF_3	406.66	0.010714	0.092025	-877.595911	-875.929684	-876.599371	-876.005770	-876.675457	-876.572718	-0.028095
TMU	399.17	0.011108	0.171896	-382.335463	-381.238795	-381.705487	-381.344430	-381.811122	-381.628118	-0.011660
TMU-BF_3	488.78	0.014977	0.187062	-706.846172	-705.052255	-705.886120	-705.175387	-706.009252	-705.807213	-0.027148
DMF	320.68	0.007126	0.100010	-248.408996	-247.717237	-248.016541	-247.780572	-248.079876	-247.972740	-0.008692
DMF-BF_3	437.68	0.011329	0.114970	-572.915438	-571.526575	-572.193704	-571.607523	-572.274652	-572.148353	-0.027743
Py	282.30	0.005283	0.086640	-248.186196	-247.482313	-247.744993	-247.550124	-247.812804	-247.720881	-0.008671
Py-BF_3	392.85	0.009404	0.101617	-572.701742	-571.304463	-571.933296	-571.388143	-572.016976	-571.905955	-0.022666
TEA	382.60	0.010465	0.200467	-292.278063	-291.328579	-291.723350	-291.443615	-291.838386	-291.627454	-0.006319
TEA-BF_3	456.49	0.013833	0.217667	-616.803091	-615.161538	-615.921490	-615.292108	-616.052060	-615.820560	-0.017090

Note that the high-level correction (HLC) of G3 theory does not affect these complexation enthalpies (as the total number of valence α and β electrons is unchanged for a Lewis acid/base complexation) and hence was omitted from the G3(MP2)RAD energy.

Table S13. Comparison of gas-phase and solution-phase energies for BF_3 complexation reactions.

Complexing species	Theory: Gas-phase			Theory: Solution-phase				Experiment	
	ΔH_{bind}	ΔH_{bind}(rel)	Absolute Deviation	ΔG_{solv}(corr)	ΔH_{solv}(corr)	ΔH_{bind}	Absolute Deviation	ΔH_{bind}	ΔH_{bind}(rel)
NB	-19.7	39.0	4.0	-26.3	-16.8	-36.5	0.7	-35.8	43.0
NM	-19.6	39.2	2.0	-28.0	-18.5	-38.0	0.4	-37.6	41.2
ACN	-26.3	32.4	14.0	-38.5	-29.0	-55.3	5.1	-60.4	18.4
PC	-35.2	23.5	8.9	-35.7	-26.2	-61.4	2.8	-64.2	14.6
MAc	-51.7	7.0	1.0	-27.6	-18.1	-69.9	2.9	-72.8	6.0
ACP	-51.7	7.0	2.7	-30.0	-20.5	-72.2	2.3	-74.5	4.3
EAc	-53.9	4.9	1.7	-29.4	-19.9	-73.8	1.8	-75.6	3.2
AC	-51.4	7.4	4.6	-31.7	-22.2	-73.6	2.4	-76.0	2.8
DE	-58.7	0.0	0.0	-29.6	-20.1	-78.8	0.0	-78.8	0.0
THP	-69.8	-11.1	4.5	-28.5	-19.0	-88.8	3.4	-85.4	-6.6
THF	-73.5	-14.7	3.1	-31.3	-21.8	-95.3	4.9	-90.4	-11.6
ISO	-66.1	-7.4	4.4	-33.6	-24.1	-90.2	0.4	-90.6	-11.8
TMPy	-84.3	-25.6	3.4	-25.0	-15.5	-99.8	1.2	-101.0	-22.2
DMSO	-76.1	-17.3	9.2	-40.6	-31.1	-107.2	1.9	-105.3	-26.5
TMU	-83.9	-25.1	4.7	-38.2	-28.7	-112.6	4.0	-108.6	-29.8
DMF	-74.7	-16.0	15.7	-47.6	-38.1	-112.8	2.3	-110.5	-31.7
Py	-99.6	-40.8	8.5	-34.3	-24.8	-124.4	3.7	-128.1	-49.3
TEA	-120.7	-61.9	1.2	-25.9	-16.4	-137.0	2.5	-139.5	-60.7

Note that ΔG_{solv}(corr) is the Gibbs free energy of solvation correction for each respective complexation reaction (calculated from G_{solv}). ΔH_{solv}(corr) is obtained by using the diethyl ether (DE) reaction as a reference to obtain $T\Delta S_{solv}$, which is assumed to be invariant for all ligands in the test set.

8.2 Benchmarking: Addition rate coefficients

Table S14. Raw energies for benchmarking rate calculations

Species	Thermal Corrections (25 or 23 °C)			Raw Energies					Thermochemistry (25 or 23 °C)	
	S (J/mol K)	Thermal correction	ZPVE	M06-2X/ 6-31+G(d,p)	R(O)MP2/ 6-31G(d)	R(O)MP2/ GTMP2Large	URCCSD(T)/ 6-31G(d)	G3(MP2)-RAD	ΔG_{solv}	$G_{solution}$
MMA (25 °C)	365.55	0.009021	0.120680	-345.650467	-344.705919	-345.108544	-344.791742	-345.194367	-0.003020	-345.109197
MMA (23 °C)	364.65	0.008869	0.120680	-345.650467	-344.705919	-345.108544	-344.791742	-345.194367	-0.003046	-345.108924
nBA	430.27	0.011651	0.176280	-424.240124	-423.036458	-423.541787	-423.155347	-423.660676	-0.008238	-423.529844
tBA	412.22	0.011485	0.174944	-424.248588	-423.047530	-423.552026	-423.165351	-423.669847	-0.004722	-423.534952
tBMA	444.75	0.013003	0.202147	-463.549392	-462.218803	-462.775432	-462.352008	-462.908637	-0.005124	-462.749116
Cumyl rad (23 °C)	384.22	0.009836	0.166563	-349.396752	-348.323496	-348.725750	-348.444085	-348.846339	-0.007672	-348.720953
Benzyl rad (23 °C)	314.74	0.006657	0.111606	-270.798030	-269.983985	-270.283062	-270.074172	-270.373249	-0.005285	-270.295772
B rad	341.46	0.007394	0.095109	-344.787223	-343.848226	-344.203725	-343.931403	-344.286902	-0.007376	-344.230551
T rad	413.44	0.010610	0.123300	-782.238209	-780.647948	-781.138963	-780.761093	-781.252109	-0.011207	-781.176355
M rad (ACN)	402.17	0.010583	0.201084	-404.914315	-403.706338	-404.205930	-403.835341	-404.334933	-0.009124	-404.178060
M rad (Toluene)	402.17	0.010583	0.201084	-404.914315	-403.706338	-404.205930	-403.835341	-404.334933	-0.006732	-404.175668
Cumyl rad-MMA TS (23 °C)	557.87	0.018072	0.288949	-695.045669	-693.030494	-693.841697	-693.229886	-694.041089	-0.011745	-693.808739
Benzyl rad-MMA TS (23 °C)	508.97	0.015277	0.233782	-616.445776	-614.688112	-615.394351	-614.858714	-615.564953	-0.010589	-615.383892
B rad-nBA TS	624.17	0.019018	0.272092	-769.022091	-766.876390	-767.739742	-767.078393	-767.941745	-0.021270	-767.742786
T rad-nBA TS	703.62	0.022345	0.300170	-1206.474504	-1203.677603	-1204.676166	-1203.909431	-1204.907994	-0.024247	-1204.689629
M rad-nBA TS	658.43	0.021889	0.378773	-829.162511	-826.748416	-827.756596	-826.994319	-828.002499	-0.018415	-827.695023
M rad-tBA TS	625.97	0.021577	0.377500	-829.171862	-826.760636	-827.767973	-827.005268	-828.012605	-0.011817	-827.696429
M rad-tBA TS (alt)	636.16	0.021671	0.377506	-829.170111	-826.758200	-827.765766	-827.002851	-828.010418	-0.012499	-827.695981
M rad-tBMA TS	655.19	0.023108	0.404581	-868.471298	-865.932393	-866.991510	-866.192138	-867.251255	-0.011811	-866.909780

Note that the high-level correction (HLC) of G3 theory does not affect these reaction barriers (as the total number of valence α and β electrons is unchanged between the reagents and transition state) and hence was omitted from the G3(MP2)RAD energy.

8.3 Binding Energy Section

Table S15. Raw energies for different binding modes

Species	Thermal Corrections (25 °C)			Raw Energies					Thermochemistry (25 °C)		
	S (J/mol K)	Thermal correction	ZPVE	M06-2X/ 6-31+G(d,p)	RMP2/ 6-31G(d)	RMP2/ GTMP2Large	URCCSD(T)/ 6-31G(d)	G3(MP2)-RAD	ΔG_{solv}	G_{solv} (G3MP2RAD)	G_{solv} (ROMP2)
MMMP	602.36	0.020071	0.330638	-1187.278112	-1184.488824	-1185.479529	-1184.723569	-1185.714274	-0.018558	-1185.450527	-1185.215782
DMPA	570.66	0.018452	0.277878	-844.672012	-842.340637	-843.263130	-842.545990	-843.468484	-0.015680	-843.252637	-843.047284
MMA	365.55	0.009021	0.120680	-345.650467	-344.705919	-345.108544	-344.791742	-345.194367	-0.004463	-345.110640	-345.024817
$AlCl_3$(MMA)	542.91	0.015729	0.127474	-1968.813652	-1965.769313	-1966.495700	-1965.904088	-1966.630474	-0.017316	-1966.566239	-1966.431465
$ZnCl_2(MMA)_2$	699.60	0.024243	0.246524	-3390.883191	-3386.584399	-3388.181307	-3386.769000	-3388.365907	-0.027372	-3388.201958	-3388.017357
[$AlCl_3$(MMMP)]	765.29	0.026781	0.337809	-2810.444577	-2805.557612	-2806.872057	-2805.839909	-2807.154354	-0.031038	-2806.907708	-2806.625411
thioether-bound [$AlCl_3$(MMMP)]	768.55	0.027055	0.336830	-2810.425985	-2805.539192	-2806.858751	-2805.820721	-2807.140280	-0.028386	-2806.892057	-2806.610527
(amine,ketone)-bound [$AlCl_3$(MMMP)]	725.12	0.025914	0.339912	-2810.436168	-2805.543606	-2806.864871	-2805.825099	-2807.146364	-0.041675	-2806.904558	-2806.623065
ketone-bound [$AlCl_3$(MMMP)]	753.44	0.026741	0.337412	-2810.444508	-2805.553624	-2806.871314	-2805.837039	-2807.154729	-0.030689	-2806.906825	-2806.623411
(ether,amine,ketone)-bound [$AlCl_3$(MMMP)]	695.40	0.025253	0.340928	-2810.416415	-2805.523700	-2806.845914	-2805.804061	-2807.126275	-0.046216	-2806.885280	-2806.604919
amine-bound [$AlCl_3$(MMMP)]	716.44	0.025838	0.339761	-2810.427218	-2805.534196	-2806.856181	-2805.815870	-2807.137856	-0.044104	-2806.897720	-2806.616045
[$AlCl_3$(DMPA)]	720.34	0.025276	0.284481	-2467.842865	-2463.410466	-2464.657625	-2463.664251	-2464.911411	-0.031652	-2464.715108	-2464.461322
(ether,ketone)-bound [$AlCl_3$(DMPA)]	711.79	0.024870	0.285295	-2467.837763	-2463.407874	-2464.655327	-2463.660015	-2464.907468	-0.033619	-2464.711752	-2464.459612
ether-bound [$AlCl_3$(DMPA)]	689.57	0.024535	0.285407	-2467.824199	-2463.392082	-2464.643636	-2463.643506	-2464.895059	-0.025063	-2464.688486	-2464.437063
[$ZnlCl_2$(MMMP)]	706.04	0.024967	0.336494	-3886.858673	-3881.659540	-3883.440491	-3881.907522	-3883.688472	-0.042613	-3883.449801	-3883.201820
(ether,amine,ketone)-bound [$ZnlCl_2$(MMMP)]	713.23	0.025214	0.336111	-3886.853392	-3881.655031	-3883.432346	-3881.902735	-3883.680051	-0.041690	-3883.441408	-3883.193704
(ether,amine)-bound	702.67	0.025203	0.336470	-3886.848976	-3881.650111	-3883.434332	-3881.894880	-3883.679101	-0.037369	-3883.434592	-3883.189824

$[ZnlCl_2(MMMP)]$											
ketone-bound $[ZnlCl_2(MMMP)(MMA)]$	963.47	0.035583	0.456458	-4232.515567	-4226.371787	-4228.555177	-	-	-0.037949	-	-4228.210497
amine-bound $[ZnlCl_2(MMMP)(MMA)]$	881.95	0.034289	0.459468	-4232.521838	-4226.376504	-4228.564660	-	-	-0.038132	-	-4228.209189
thioether-bound $[ZnlCl_2(MMMP)(MMA)]$	912.04	0.035304	0.456546	-4232.512722	-4226.370782	-4228.565671	-	-	-0.037160	-	-4228.214551
ether-bound $[ZnlCl_2(MMMP)(MMA)]$	972.59	0.035595	0.456848	-4232.519947	-4226.364165	-4228.560485	-	-	-0.037259	-	-4228.215748
$[ZnCl_2(DMPA)]$	711.79	0.024870	0.285295	-2467.837763	-2463.407874	-2464.655327	-2463.660015	-2464.907468	-0.033619	-2464.711752	-2464.459612
ketone-bound $[ZnCl_2(DMPA)(MMA)]$	909.54	0.033827	0.403842	-3889.910824	-3884.228147	-3886.343165	-	-	-0.033914	-	-3886.042696
$[AlCl_2(MMMP)]^+$	664.57	0.023615	0.339741	-2350.025592	-2345.708061	-2346.914964	-2345.975204	-2347.182107	-0.085663	-2346.979882	-2346.712739
$[AlCl_2(MMMP)][AlCl_3]$	885.38	0.032847	0.346408	-4433.607996	-4426.619927	-4428.262442	-	-	-0.052524	-	-4428.036253
ketone-amine bound $[AlCl_2(MMMP)]^+$	671.46	0.023803	0.339150	-2350.017002	-2345.695196	-2346.906256	-2345.963940	-2347.175000	-0.081761	-2346.970058	-2346.701314
$[AlCl_2(DMPA)]^+$	667.31	0.023011	0.284144	-2007.405172	-2003.546268	-2004.684512	-2003.785039	-2004.923283	-0.072323	-2004.764230	-2004.525459
$[AlCl_2(DMPA)(MMA)]^+$	858.31	0.032357	0.407020	-2353.108902	-2348.300757	-2349.845112	-	-	-0.068107	-	-2349.571311
$[AlCl_2(MMA)_2]^+$	699.41	0.023434	0.248929	-1854.051592	-1850.630189	-1851.655561	-1850.836511	-1851.861883	-0.066731	-1851.735675	-1851.529354
$[AlCl_2(MMA)_3]^+$	868.69	0.032578	0.371562	-2199.739293	-2195.367476	-2196.799425	-	-	-0.062218	-	-2196.556151

Note that the high-level correction (HLC) of G3 theory does not affect these complexation free-energies (as the total number of valence α and β electrons is unchanged for a Lewis acid/base complexation) and hence was omitted from the G3(MP2)RAD energy.

8.4 BDE and Rate Coefficient Section

Table S16. Raw energies for rate coefficient calculations

Species	Thermal Corrections (25 °C)			Raw Energies					Thermochemistry (25 °C)		
	S (J/mol K)	Thermal correction	ZPVE	M06-2X/ 6-31+G(d,p)	R(O)MP2/ 6-31G(d)	R(O)MP2/ GTMP2Large	URCCSD(T)/ 6-31G(d)	G3(MP2)-RAD	ΔG_{solv}	G_{solv} (G3MP2RAD)	H_{gas} (G3MP2RAD)
B rad	341.30	0.007389	0.095114	-344.787224	-343.848235	-344.203722	-343.931413	-344.286899	-0.006929	-344.230082	-344.184396
MMA	365.55	0.009021	0.120680	-345.650467	-344.705919	-345.108544	-344.791742	-345.194367	-0.004463	-345.110640	-345.064665
B rad-MMA TS	561.71	0.016600	0.216130	-690.433991	-688.548285	-689.308189	-688.717064	-689.476969	-0.015320	-689.323345	-689.244238
B rad-MMA	533.76	0.015947	0.219727	-690.488281	-688.602252	-689.359410	-688.769362	-689.526520			-689.290845
B rad $AlCl_3$	518.56	0.014153	0.101758	-1967.930440	-1964.892564	-1965.568416	-1965.026550	-1965.702402	-0.020395	-1965.665774	-1965.586492
B rad/$AlCl_3$-MMA TS	692.54	0.023132	0.222785	-2313.587242	-2309.599415	-2310.686303	-2309.817939	-2310.904827	-0.023847	-2310.761403	-2310.658911
B rad/$AlCl_3$-MMA	681.34	0.022663	0.226010	-2313.656664	-2309.668447	-2310.752402	-2309.884389	-2310.968344			-2310.719671
MMA $AlCl_3$	542.91	0.015729	0.127474	-1968.813652	-1965.769313	-1966.495700	-1965.904088	-1966.630474	-0.017316	-1966.566239	-1966.487271
B rad-MMA/$AlCl_3$ TS	694.35	0.023125	0.223165	-2313.611658	-2309.622878	-2310.712468	-2309.838726	-2310.928317	-0.022439	-2310.783315	-2310.682027
B rad-MMA/$AlCl_3$	688.97	0.022651	0.226336	-2313.657454	-2309.667416	-2310.752340	-2309.883547	-2310.968471			-2310.719484
T rad	413.44	0.010610	0.123300	-782.238209	-780.647948	-781.138963	-780.761093	-781.252109	-0.010171	-781.175319	-781.118198
T rad-MMA TS	636.66	0.019900	0.244256	-1127.884981	-1125.348187	-1126.243626	-1125.546955	-1126.442395	-0.018558	-1126.269096	-1126.178239
T rad-MMA	609.37	0.019264	0.247834	-1127.939480	-1125.402486	-1126.295079	-1125.599616	-1126.492209			-1126.225111
T rad $AlCl_3$	589.23	0.017367	0.129998	-2405.384028	-2401.694019	-2402.505817	-2401.858182	-2402.669980	-0.023904	-2402.613432	-2402.522616
T rad/$AlCl_3$-MMA TS	760.51	0.026362	0.251036	-2751.040905	-2746.401302	-2747.624169	-2746.650107	-2747.872974	-0.026862	-2747.708802	-2747.595577
T rad/$AlCl_3$-MMA	750.15	0.025920	0.254239	-2751.109424	-2746.469595	-2747.689454	-2746.715647	-2747.935506			-2747.655347
T rad -MMA/$AlCl_3$ TS	768.69	0.026417	0.251261	-2751.063241	-2746.423167	-2747.649060	-2746.668887	-2747.894781	-0.025546	-2747.729942	-2747.617103
T rad-MMA/$AlCl_3$	764.49	0.025838	0.254880	-2751.109115	-2746.468831	-2747.688609	-2746.715007	-2747.934785			-2747.654067
D rad	449.98	0.012255	0.176273	-499.767922	-498.364925	-498.930929	-498.496564	-499.062568	-0.008673	-498.933813	-498.874040
D rad-MMA TS	618.84	0.020692	0.298430	-845.419854	-843.073427	-844.046867	-843.285365	-844.258805	-0.014638	-844.024596	-843.939683
D rad-MMA	603.65	0.020302	0.301443	-845.462467	-843.121530	-844.088983	-843.331062	-844.298515			-843.976770
D rad $AlCl_3$	601.85	0.018921	0.183154	-2122.929456	-2119.427627	-2120.317073	-2119.607259	-2120.496706	-0.017711	-2120.380687	-2120.294630
D rad/$AlCl_3$-MMA TS	746.36	0.027018	0.305604	-2468.574859	-2464.130702	-2465.428457	-2464.390783	-2465.688538	-0.023313	-2465.463985	-2465.355916
D rad/$AlCl_3$-MMA	763.51	0.026880	0.308695	-2468.620555	-2464.180456	-2465.472592	-2464.437691	-2465.729827			-2465.394251

D rad-MMA/$AlCl_3$ TS	763.63	0.027402	0.305279	-2468.600413	-2464.152017	-2465.452358	-2464.411404	-2465.711745	-0.024997	-2465.490778	-2465.379064
D rad-MMA/$AlCl_3$	746.74	0.026814	0.308656	-2468.637439	-2464.193869	-2465.488842	-2464.451637	-2465.746610			-2465.411140
M rad	402.17	0.010583	0.201084	-404.914315	-403.706338	-404.205930	-403.835341	-404.334933	-0.008008	-404.176944	-404.123266
M rad-MMA TS	580.47	0.019219	0.322998	-750.571741	-748.417283	-749.323171	-748.629806	-749.535694	-0.014038	-749.273434	-749.193477
M rad-MMA	575.01	0.018701	0.326234	-750.607405	-748.458075	-749.359101	-748.668044	-749.569070			-749.224135
M rad (N) $AlCl_3$	546.74	0.016777	0.208824	-2028.078688	-2024.771739	-2025.595907	-2024.947616	-2025.771783	-0.020288	-2025.628558	-2025.546182
Nbound M rad/$AlCl_3$-MMA TS	693.10	0.024940	0.332028	-2373.726096	-2369.474656	-2370.706580	-2369.734398	-2370.966322	-0.024443	-2370.712504	-2370.609353
Nbound M rad/$AlCl_3$-MMA	691.70	0.024636	0.335542	-2373.765911	-2369.516313	-2370.745740	-2369.772900	-2371.002327			-2370.642150
M rad (O) $AlCl_3$	565.77	0.017330	0.208099	-2028.080645	-2024.775681	-2025.597539	-2024.952304	-2025.774162	-0.020516	-2025.633498	-2025.548733
Obound M rad/$AlCl_3$-MMA TS	732.05	0.025784	0.330431	-2373.738762	-2369.488634	-2370.717790	-2369.748628	-2370.977784	-0.025150	-2370.729850	-2370.621569
Obound M rad/$AlCl_3$-MMA	724.97	0.025219	0.333560	-2373.775442	-2369.528580	-2370.754180	-2369.785909	-2371.011509			-2370.652730
M rad-MMA/$AlCl_3$	722.94	0.025227	0.333306	-2373.781299	-2369.526744	-2370.755516	-2369.786505	-2371.015277			-2370.656744

Note that the high-level correction (HLC) of G3 theory does not affect these activation free-energies and reaction enthalpies (as the total number of valence α and β electrons is unchanged for a Lewis acid/base complexation) and hence was omitted from the G3(MP2)RAD energy.

Table S17. Raw energies for RSE calculations

Species	Thermal Corrections (25 °C)			Raw Energies					Thermochemistry (25 °C)
	S (J/mol K)	Thermal correction	ZPVE	M06-2X/ 6-31+G(d,p)	R(O)MP2/ 6-31G(d)	R(O)MP2/ GTMP2Large	URCCSD(T)/ 6-31G(d)	G3(MP2)-RAD	H_{gas} (G3MP2RAD)
B rad	341.30	0.007389	0.095114	-344.787224	-343.848235	-344.203722	-343.931413	-344.469715	-344.367212
B rad-H	334.83	0.007369	0.107168	-345.439091	-344.485843	-344.852650	-344.571887	-345.126953	-345.012416
B rad ACl_3	518.56	0.014153	0.101758	-1967.930440	-1964.892564	-1965.568416	-1965.026550	-1965.998174	-1965.882264
B rad-H ACl_3	504.71	0.014004	0.114358	-1968.601213	-1965.550064	-1966.238592	-1965.684870	-1966.674614	-1966.546252
H rad	114.61	0.002360	0.000000	-0.496666	-0.498233	-0.499818	-0.498233	-0.501706	-0.499345
CH_3 rad	195.80	0.004085	0.028920	-39.811897	-39.668535	-39.730543	-39.690991	-39.785206	-39.752201
CH_3 rad-H	206.77	0.003816	0.043703	-40.487943	-40.332551	-40.404220	-40.355875	-40.465196	-40.417676
D rad	449.98	0.012255	0.176273	-499.767922	-498.364925	-498.930929	-498.496564	-499.339514	-499.150986
D rad-H	433.99	0.011891	0.189919	-500.415926	-499.005928	-499.580377	-499.136326	-499.993165	-499.791355
D rad $AlCl_3$	601.85	0.018921	0.183154	-2122.929456	-2119.427627	-2120.317073	-2119.607259	-2120.886608	-2120.684532
D rad-H $AlCl_3$	587.37	0.018539	0.196961	-2123.584132	-2120.075679	-2120.974497	-2120.253491	-2121.547656	-2121.332156
$AlCl_3$	313.68	0.006284	0.004708	-1623.103072	-1621.008010	-1621.330528	-1621.057238	-1621.492713	-1621.481720
T rad	413.79	0.010604	0.123361	-782.238338	-780.648035	-781.139101	-780.761178	-781.491537	-781.357572
T rad-H	408.62	0.010624	0.135317	-782.889987	-781.285594	-781.787910	-781.401580	-782.148634	-782.002692
M rad	402.17	0.010583	0.201084	-404.914315	-403.706338	-404.205930	-403.835341	-404.583640	-404.371973
M rad-H	391.58	0.010352	0.214137	-405.567743	-404.351319	-404.860483	-404.480227	-405.243542	-405.019054
T rad $AlCl_3$	589.23	0.017367	0.129998	-2405.384028	-2401.694019	-2402.505817	-2401.858182	-2403.022230	-2402.874866
T rad-H $AlCl_3$	574.86	0.017245	0.142583	-2406.055013	-2402.351839	-2403.176105	-2402.516745	-2403.698705	-2403.538877
M rad (N) $AlCl_3$	546.74	0.016777	0.208824	-2028.078688	-2024.771739	-2025.595907	-2024.947616	-2026.133446	-2025.907845
M rad (O) $AlCl_3$	565.77	0.017330	0.208099	-2028.080645	-2024.775681	-2025.597539	-2024.952304	-2026.135825	-2025.910396
M rad-H (N) $AlCl_3$	522.18	0.016415	0.223060	-2028.735891	-2025.419603	-2026.255069	-2025.595355	-2026.797928	-2026.558453
M rad-H (O) $AlCl_3$	550.98	0.017038	0.221244	-2028.736333	-2025.422674	-2026.253945	-2025.599285	-2026.797662	-2026.559380

Note that these G3(MP2)RAD energies are high-level correction (HLC) inclusive.

Table S18. Raw energies for Electron affinity and ionization energy calculations

Species	Thermal Corrections (25 °C)			Raw Energies					Thermochemistry (25 °C)
	S (J/mol K)	Thermal correction	ZPVE	M06-2X/ 6-31+G(d,p)	R(O)MP2/ 6-31+G(d)	R(O)MP2/ GTMP2Large	URCCSD(T)/ 6-31+G(d)	G3(MP2)-RAD(+)	H_{gas} (G3MP2RAD)
M cation	400.68	0.010573	0.203841	-404.735646	-403.568574	-404.033509	-403.697117	-404.406790	-404.192376
M rad	402.17	0.010583	0.201084	-404.914315	-403.733364	-404.205930	-403.864430	-404.585703	-404.374037
MMA	365.55	0.009021	0.120680	-345.650467	-344.726858	-345.108544	-344.813513	-345.383459	-345.253757
MMA radanion	389.41	0.009786	0.115746	-345.641234	-344.704106	-345.096502	-344.787083	-345.371708	-345.246176
MMA($AlCl_3$)	542.91	0.015729	0.127474	-1968.813652	-1965.799161	-1966.495700	-1965.936137	-1966.933892	-1966.790689
MMA($AlCl_3$) radanion	534.17	0.015911	0.124026	-1968.884253	-1965.856072	-1966.562004	-1965.990299	-1967.001417	-1966.861480
B rad	341.30	0.007389	0.095114	-344.787224	-343.870141	-344.203722	-343.953287	-344.469684	-344.367181
B cation	327.28	0.007225	0.096723	-344.547660	-343.644801	-343.976416	-343.724017	-344.234480	-344.130532
D rad	449.98	0.012255	0.176273	-499.767922	-498.397300	-498.930929	-498.529666	-499.340240	-499.151713
D cation	420.01	0.011715	0.179823	-499.562992	-498.207011	-498.733102	-498.335561	-499.134629	-498.943091
B rad $AlCl_3$	518.56	0.014153	0.101758	-1967.930440	-1964.922114	-1965.568416	-1965.057424	-1965.999498	-1965.883587
B cation $AlCl_3$	542.28	0.014842	0.101946	-1967.662156	-1964.673626	-1965.321126	-1964.802389	-1965.741692	-1965.624903
T rad	413.79	0.010604	0.123361	-782.238338	-780.673569	-781.139101	-780.787242	-781.492068	-781.358103
T cation	402.49	0.010417	0.124959	-782.011626	-780.459058	-780.923495	-780.569616	-781.269379	-781.134003
D rad $AlCl_3$	601.85	0.018921	0.183154	-2122.929456	-2119.475116	-2120.317073	-2119.656953	-2120.888812	-2120.686737
D cation $AlCl_3$	580.20	0.018642	0.185330	-2122.685999	-2119.248453	-2120.084427	-2119.426371	-2120.648278	-2120.444307
M rad (O) $AlCl_3$	565.77	0.017330	0.208099	-2028.080645	-2024.814259	-2025.597539	-2024.994312	-2026.139255	-2025.913826
M cation (O) $AlCl_3$	533.17	0.016258	0.210676	-2027.880225	-2024.626910	-2025.404348	-2024.804551	-2025.939683	-2025.712749
T rad $AlCl_3$	589.23	0.017367	0.129998	-2405.384028	-2401.727169	-2402.505817	-2401.893740	-2403.024638	-2402.877273
T cation $AlCl_3$	610.38	0.018077	0.130146	-2405.124873	-2401.487433	-2402.266894	-2401.647545	-2402.775287	-2402.627064
M rad (N) $AlCl_3$	546.74	0.016777	0.208824	-2028.078688	-2024.809344	-2025.595907	-2024.988215	-2026.136440	-2025.910839
M cation (N) $AlCl_3$	568.17	0.017666	0.209503	-2027.846062	-2024.592748	-2025.372627	-2024.771082	-2025.908655	-2025.681486

Note that these G3(MP2)RAD(+) energies are high-level correction (HLC) inclusive. Note that "cation" corresponds to the 1-electron oxidized form of the parent radical, i.e. the B cation is an oxidized B radical (an acylium cation). Likewise "radanion" corresponds to the reduced form MMA, i.e. MMA rad anion is the species formed from the 1-electron reduction of neutral MMA.

9. Gas-phase Geometries of all species in this study

9.1 Benchmarking: BF_3 binding enthalpies

BF_3

1\1\GINC-R38\Freq\RM062X\6-31+G(d,p)\B1F3\ROOT\13-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM0
62X/6-31+G(d,p) Freq\\BF3.freq\\0,1\B,0.,0.,0.\F,0.6580190558,-1.139722437,0.\F,0.6580190558,1.139722437,0.\F,-1.3160381117,0.,0.\\
Version=ES64L-G09RevD.01\State=1-A1'\HF=-324.4698495\RMSD=1.026e-09\RMSF=4.303e-07\ZeroPoint=0.0125213\Thermal=0.016027
8\Dipole=0.,0.,0.\PG=D03H [O(B1),3C2(F1)]\\@

NB

1\1\GINC-R86\Freq\RM062X\6-31+G(d,p)\C6H5N1O2\ROOT\11-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenCh
k RM062X/6-31+G(d,p) Freq\\PhNO2.freq\\0,1\N,0.,0.,1.6305885102\C,0.,0.,0.1550626477\C,0.,1.2202812164,-0.5090268649\C,0.,1.210
6653261,-1.9008135358\C,0.,0.,-2.5940015806\C,0.,-1.2106653261,-1.9008135358\C,0.,-1.2202812164,-0.5090268649\H,0.,2.141612568
1,0.0604963786\H,0.,2.1500228376,-2.4430284134\H,0.,0.,-3.6792262441\H,0.,-2.1500228376,-2.4430284134\H,0.,-2.1416125681,0.060
4963786\O,0.,-1.0795718488,2.1943707689\O,0.,1.0795718488,2.1943707689\\Version=ES64L-G09RevD.01\State=1-A1\HF=-436.586284
9\RMSD=2.218e-09\RMSF=1.707e-05\ZeroPoint=0.1044305\Thermal=0.1111892\Dipole=0.,0.,-1.9050218\PG=C02V [C2(H1C1C1N1),SGV(
C4H4O2)]\\@

NB-BF_3

1\1\GINC-R43\Freq\RM062X\6-31+G(d,p)\C6H5B1F3N1O2\ROOT\12-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test G
enChk RM062X/6-31+G(d,p) Freq\\Nitrobenzene-BF3.CS.freq\\0,1\C,0.,1.4948872829,3.1079262522\C,0.,0.4600654663,4.0439735999\C,
0.,-0.8733723861,3.6311262115\C,0.,-1.1839829769,2.2764408034\C,0.,-0.1306910509,1.367697338\C,0.,1.2079706939,1.7471389294\
N,0.,-0.463768282,-0.0542517298\O,0.,0.5094308395,-0.8410904465\O,0.,-1.6100346737,-0.4049084779\H,0.,2.528263562,3.43601637
77\H,0.,0.6941100502,5.103516382\H,0.,-1.6724283465,4.3639501034\H,0.,-2.2078656149,1.9222904849\H,0.,1.98833269,0.996252969
1\B,0.,0.1896082315,-2.5877801016\F,1.1511396344,-0.4994926872,-2.748458224\F,0.,1.4716698892,-3.0069622478\F,-1.1511396344,-
0.4994926872,-2.748458224\\Version=ES64L-G09RevD.01\State=1-A'\HF=-761.0700641\RMSD=3.619e-09\RMSF=3.979e-05\ZeroPoint=0.
118421\Thermal=0.1297792\Dipole=0.,0.1246891,3.7880047\PG=CS [SG(C6H5B1F1N1O2),X(F2)]\\@

ACN

1\1\GINC-R197\Freq\RM062X\6-31+G(d,p)\C2H3N1\ROOT\12-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk
RM062X/6-31+G(d,p) Freq\\ACN.freq\\0,1\N,0.,0.,-1.3238859927\C,0.,0.,-0.1684597342\C,0.,0.,1 .2942494604\H,0.5132889505,0.889042
5413,1.6641408393\H,0.5132889505,-0 .8890425413,1.6641408393\H,-1.026577901,0.,1.6641408393\\Version=ES64L -G09RevD.01\Stat
e=1-A1\HF=-132.7007779\RMSD=1.464e-09\RMSF=1.008e-05\Z eroPoint=0.0458374\Thermal=0.0494376\Dipole=0.,0.,1.5798513\PG =C0
3V [C3(C1C1N1),3SGV(H1)]\\@

ACN-BF_3

1\1\GINC-R85\Freq\RM062X\6-31+G(d,p)\C2H3B1F3N1\ROOT\12-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenC
hk RM062X/6-31+G(d,p) Freq\\ACN-BF3.freq\\0,1\B,0.5672959498,1.3917857483,2.6992838088\F,1.3044695709,0.9807009364,1.63636
39022\F,-0.7750551512,1.2271715654,2.5848317472\F,1.09237737,1.1207936998,3.9211895544\N,0.732542355,3.1371282237,2.60774
13294\C,0.8413567214,4.2761842145,2.5483278217\C,0.9785068007,5.7249063071,2.4728329049\H,0.5362372987,6.1751050848,3.36
27911651\H,0.4641208494,6.0892787231,1.5823515962\H,2.0369482353,5.983625497,2.41751617\\Version=ES64L-G09RevD.01\State=
1-A\HF=-457.186686\RMSD=2.797e-09\RMSF=2.610e-05\ZeroPoint=0.0601023\Thermal=0.0681151\Dipole=0.3281471,3.4574778,-0.180
7892\PG=C01 [X(C2H3B1F3N1)]\\@

ACP

1\1\GINC-R48\Freq\RM062X\6-31+G(d,p)\C8H8O1\ROOT\11-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\Acetophenone.freq\\0,1\C,0.0026779007,0.,-0.0285691475\C,-0.0179999392,0.,1.3693838722\C,1.1759474334,0.,2.0882469858\C,2.3947520215,0.,1.4130596218\C,2.4209394469,0.,0.0170015636\C,1.2304089498,0.,-0.7002203882\C,-1.2558291268,0.,-0.8482389156\O,-1.200742466,0.,-2.0620078336\C,-2.5889332626,0.,-0.1324794473\H,-0.9619304836,0.,1.9056101179\H,1.1536660954,0.,3.1732642657\H,3.3245543025,0.,1.9734571055\H,3.370609401,0.,-0.5084130059\H,1.2238786637,0.,-1.7854547344\H,-3.3837506916,0.,-0.8775092944\H,-2.6836046048,-0.883697821,0.5059609761\H,-2.6836046048,0.883697821,0.5059609761\\Version=ES64L-G09RevD.01\State=1-A'\HF=-384.7445408\RMSD=4.369e-09\RMSF=8.078e-05\ZeroPoint=0.1390765\Thermal=0.1468716\Dipole=0.188016,0.,1.2224896\PG=CS [SG(C8H6O1),X(H2)]\\@

ACP-BF_3

1\1\GINC-R44\Freq\RM062X\6-31+G(d,p)\C8H8B1F3O1\ROOT\12-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\Acetophenone-BF3.freq\\0,1\C,-1.2414961403,0.1645030919,-0.0299698903\C,-2.2236536125,1.1581833264,0.0794871444\C,-3.5682124469,0.8045736227,0.1137827167\C,-3.9366904402,-0.5375501287,0.0282979796\C,-2.9622836913,-1.5314573693,-0.0825536919\C,-1.6181554922,-1.1851415935,-0.105955323\C,0.1950466651,0.5016241023,-0.0428097937\O,0.9959080405,-0.448955513,0.016127152\C,0.6627397114,1.9214763192,-0.0964372444\H,-1.9468272889,2.2042952041,0.1528873764\H,-4.3270539935,1.5740430072,0.2059982732\H,-4.9870503906,-0.8106352148,0.0492492779\H,-3.25312387,-2.5743514207,-0.1479931452\H,-0.8464160652,-1.9432162709,-0.1846178735\H,0.6886221031,2.3073051313,0.9294921817\H,-0.0158094864,2.5351616641,-0.6880075238\H,1.6721253453,1.9721990836,-0.5000160954\B,2.6206046937,-0.3119357842,0.074322759\F,3.026365305,-1.5921120491,0.2611327648\F,2.8454202655,0.5311870378,1.1358765875\F,2.9631807884,0.2347337537,-1.137973632\\Version=ES64L-G09RevD.01\State=1-A\HF=-709.2425533\RMSD=2.429e-09\RMSF=1.842e-05\ZeroPoint=0.1541431\Thermal=0.1660597\Dipole=-3.417964,1.0011349,-0.0877893\PG=C01 [X(C8H8B1F3O1)]\\@

EA

1\1\GINC-R62\Freq\RM062X\6-31+G(d,p)\C4H8O2\ROOT\11-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\AcOEt.1.freq\\0,1\O,0.,1.2852474641,-1.1640869812\C,0.,0.0913061029,-0.9821026197\C,0.,-0.9584102491,-2.060735959\O,0.,-0.4663254473,0.2422600518\C,0.,0.4512107478,1.3476894314\C,0.,-0.3722019869,2.6169075113\H,0.,-0.4731836304,-3.0348593619\H,-0.8820018641,-1.5942412691,-1.9544765711\H,0.8820018641,-1.5942412691,-1.9544765711\H,-0.8835259668,1.091973424,1.2711975202\H,0.8835259668,1.091973424,1.2711975202\H,-0.8868439596,-1.0088253218,2.6641467809\H,0.,0.2883933386,3.4878324693\H,0.8868439596,-1.0088253218,2.6641467809\\Version=ES64L-G09RevD.01\State=1-A'\HF=-307.5834427\RMSD=1.634e-09\RMSF=6.730e-05\ZeroPoint=0.1193629\Thermal=0.1267239\Dipole=0.,-0.6992286,0.4123689\PG=CS [SG(C4H2O2),X(H6)]\\@

EA-BF_3

1\1\GINC-R43\Freq\RM062X\6-31+G(d,p)\C4H8B1F3O2\ROOT\12-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\AcOEt-BF3.1.freq\\0,1\B,0.1755006028,-1.016912547,-2.4261519261\F,-0.0538908667,-2.0595634313,-1.5632823101\F,-0.8430177133,-0.8233483739,-3.3259667816\F,1.4253013218,-0.9601882968,-2.9459039178\O,0.1167775196,0.3113441745,-1.4689126378\C,-0.8789569964,0.6327757786,-0.8008779026\C,-2.1763974809,-0.1016830254,-0.7334542134\O,-0.8345332188,1.7126651141,-0.0680896984\C,0.3961569553,2.4881687756,-0.0765905991\C,0.1788977062,3.6674139647,0.8415433989\H,-2.970639008,0.5765121201,-1.0538616278\H,-2.1552001958,-0.9882956191,-1.3602036904\H,-2.3626895017,-0.3720532184,0.3084887934\H,0.5961217058,2.7864464676,-1.1082412163\H,1.2050836476,1.8349194247,0.2580897698\H,-0.6481050237,4.2874991681,0.4889533868\H,1.0846509659,4.2779336696,0.864158126\H,-0.0391204196,3.3333958541,1.8582630464\\Version=ES64L-G09RevD.01\State=1-A\HF=-632.0808718\RMSD=2.207e-09\RMSF=1.262e-05\ZeroPoint=0.134269\Thermal=0.1448233\Dipole=-0.8699476,2.1293948,1.87786\PG=C01 [X(C4H8B1F3O2)]\\@

AC

1\1\GINC-R38\Freq\RM062X\6-31+G(d,p)\C3H6O1\ROOT\12-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\Acetone.C2.freq\\0,1\O,0.,-1.3034282064,0.\C,0.,-0.0919041168,0.\C,1.2880145479,0.7039859184,-0.0008700022\C,-1.2880145479,0.7039859184,0.0008700022\H,1.2938004775,1.418388458,-0.830060224\H,2.1405865327,0.029943201,-0.0812033009\H,1.3630399329,1.2840235841,0.9249446324\H,-2.1405865327,0.029943201,0.0812033009\H,-1.3630399329,1.2840235841,-0.9249446324\H,-1.2938004775,1.418388458,0.830060224\\Version=ES64L-G09RevD.01\State=1-A\HF=-193.0719045\RMSD=2.648e-09\RMSF=6.829e-05\ZeroPoint=0.0843947\Thermal=0.0897888\Dipole=0.,1.2347162,0.\PG=C02 [C2(C1O1),X(C2H6)]\\@

AC-BF_3

1\1\GINC-R38\Freq\RM062X\6-31+G(d,p)\C3H6O1\ROOT\12-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\Acetone.C2.freq\\0,1\O,0.,-1.3034282064,0.\C,0.,-0.0919041168,0.\C,1.2880145479,0.7039859184,-0.0008700022\C,-1.2880145479,0.7039859184,0.0008700022\H,1.2938004775,1.418388458,-0.830060224\H,2.1405865327,0.029943201,-0.0812033009\H,1.3630399329,1.2840235841,0.9249446324\H,-2.1405865327,0.029943201,0.0812033009\H,-1.3630399329,1.2840235841,-0.9249446324\H,-1.2938004775,1.418388458,0.830060224\\Version=ES64L-G09RevD.01\State=1-A\HF=-193.0719045\RMSD=2.648e-09\RMSF=6.829e-05\ZeroPoint=0.0843947\Thermal=0.0897888\Dipole=0.,1.2347162,0.\PG=C02 [C2(C1O1),X(C2H6)]\\@

DE

1\1\GINC-R44\Freq\RM062X\6-31+G(d,p)\C4H10O1\ROOT\11-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\Et2O.4.freq\\0,1\O,0.,-0.2374380755,0.\C,0.,0.5420636117,-1.1757889122\C,0.,0.5420636117,1.1757889122\C,0.,-0.3899761383,2.3703870156\C,0.,-0.3899761383,-2.3703870156\H,0.8883770585,1.1941680164,-1.1909573993\H,-0.8883770585,1.1941680164,-1.1909573993\H,-0.8883770585,1.1941680164,1.1909573993\H,0.8883770585,1.1941680164,1.1909573993\H,-0.8862720629,-1.0288343942,2.3510626424\H,0.,0.18220932,3.3022405789\H,0.8862720629,-1.0288343942,2.3510626424\H,0.8862720629,-1.0288343942,-2.3510626424\H,0.,0.18220932,-3.3022405789\H,-0.8862720629,-1.0288343942,-2.3510626424\\Version=ES64L-G09RevD.01\State=1-A1\HF=-233.5561438\RMSD=2.884e-10\RMSF=3.956e-05\ZeroPoint=0.1378582\Thermal=0.1446415\Dipole=0.,0.4819496,0.\PG=C02V [C2(O1),SGV(C4H2),X(H8)]\\@

DE-BF_3

1\1\GINC-R203\Freq\RM062X\6-31+G(d,p)\C4H10B1F3O1\ROOT\12-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\Et2O-BF3.1.freq\\0,1\O,-0.9766128295,-0.096065283,-0.3070466082\B,0.6021880821,0.0925140666,0.0317703545\F,0.7343301096,-0.3157119479,1.3358192989\F,0.7961713989,1.4330929095,-0.1426195481\F,1.2167219261,-0.7207429745,-0.8775577987\C,-1.8895509914,0.6621569012,0.5281868293\C,-1.4382228171,-1.4020157179,-0.7405145625\C,-1.190035216,-2.4708562928,0.304900481\C,-2.7474476552,1.5563148822,-0.3404178814\H,-1.259552857,1.2373088667,1.2069165251\H,-2.4754601954,-0.0507665121,1.1155948999\H,-0.8915210886,-1.6014405507,-1.6616049349\H,-2.4999545175,-1.2832256508,-0.9735236068\H,-0.120407061,-2.5948182309,0.4802566585\H,-1.6019987365,-3.4182171285,-0.0534114784\H,-1.6711298829,-2.2254993335,1.2553946458\H,-2.1139723278,2.2462942344,-0.9014731865\H,-3.4286332068,2.1352267309,0.2888982362\H,-3.3475921338,0.9744810312,-1.0455283238\\Version=ES64L-G09RevD.01\State=1-A\HF=-558.0573983\RMSD=3.876e-09\RMSF=3.192e-06\ZeroPoint=0.1535658\Thermal=0.1642133\Dipole=-2.3349122,-0.512638,-0.1177514\PG=C01 [X(C4H10B1F3O1)]\\@

THP

1\1\GINC-R44\Freq\RM062X\6-31+G(d,p)\C5H10O1\ROOT\12-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\THP.freq\\0,1\C,0.0006596544,0.0031126705,0.000457297\C,-0.0004333343,-0.0023358356,1.5316800689\C,1.4425093615,-0.0023411173,-0.515016986\C,2.221587688,-1.1449106774,0.12960932\C,0.8684667203,-1.1449057245,2.0489015467\O,2.1884115256,-1.0645995507,1.5428478596\H,-0.548843367,0.8669591948,-0.3869502735\H,-0.5165410537,-0.8956018274,-0.3641722585\H,-1.0178909105,-0.1046444937,1.9251384891\H,0.4068415097,0.9447767152,1.9061079709\H,1.9320071947,0.9447711326,-0.2572157182\H,1.4712616828,-0.1046536048,-1.6055223589\H,3.276938793,-1.1217668444,-0.1525073331\H,1.7997872155,-2.1135096308,-0.1915031414\H,0.4243050182,-2.1135045961,1.7595066738\H,0.9573150649,-1.1217583538,3.1376905843\\Version=ES64L-G09RevD.01\State=1-A'\HF=-271.6563634\RMSD=2.111e-09\RMSF=1.299e-05\ZeroPoint=0.147728\Thermal=0.1531194\Dipole=-0.5193007,0.0625268,-0.3661126\PG=CS [SG(C1H2O1),X(C4H8)]\\@

THP-BF_3

1\1\GINC-R341\Freq\RM062X\6-31+G(d,p)\C5H10B1F3O1\ROOT\12-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\THP-BF3.freq\\0,1\C,0.1905110387,0.,-2.9315958585\C,-0.252841856,-1.2504054978,-2.1696624554\C,-0.252841856,1.2504054978,-2.1696624554\C,0.2417012839,1.2108941312,-0.7359429729\C,0.2417012839,-1.2108941312,-0.7359429729\O,-0.2426621421,0.,-0.0919601375\H,-0.2235172276,0.,-3.9436974844\H,1.284199214,0.,-3.0296327883\H,0.1335675518,-2.1594973479,-2.6411587515\H,-1.3465089345,-1.321127084,-2.1646600747\H,-1.3465089345,1.321127084,-2.1646600747\H,0.1335675518,2.1594973479,-2.6411587515\H,-0.1465692394,2.0282612491,-0.1303344494\H,1.337054854,1.1960948939,-0.6749128619\H,1.337054854,-1.1960948939,-0.6749128619\H,-0.1465692394,-2.0282612491,-0.1303344494\B,-0.0603005637,0.,1.5365109118\F,-0.6765144287,-1.1534352461,1.9235330893\F,-0.6765144287,1.1534352461,1.9235330893\F,1.3010912187,0.,1.71121231\\Version=ES64L-G09RevD.01\State=1-A'\HF=-596.1609618\RMSD=1.461e-09\RMSF=1.135e-05\ZeroPoint=0.1632793\Thermal=0.1727621\Dipole=0.22617,0.,-2.5851797\PG=CS [SG(C1H2B1F1O1),X(C4H8F2)]\\@

THF

1\1\GINC-R40\Freq\RM062X\6-31+G(d,p)\C4H8O1\ROOT\11-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\THF.freq\\0,1\C,-5.210700019,1.0799058736,-0.1670971069\C,-4.3041622853,-0.0893414692,0.2166224536\C,-2.9347885582,0.4385645726,-0.2207436056\C,-3.0493025609,1.9145611306,0.1593079622\O,-4.4238364971,2.2587638535,-0.0054087362\H,-6.1001084043,1.165719941,0.4636406978\H,-5.5311682125,1.0021415497,-1.2150915836\H,-4.5896845938,-1.0238958606,-0.2716226353\H,-4.3207162846,-0.2449754127,1.300633299\H,-2.8169428145,0.331834541,-1.3043932366\H,-2.0958998428,-0.0606481371,0.2695128987\H,-2.4471877037,2.5741748523,-0.4720388569\H,-2.7612822233,2.0746645653,1.2073884498\\Version=ES64L-G09RevD.01\State=1-A\HF=-232.352291\RMSD=1.140e-09\RMSF=5.645e-05\ZeroPoint=0.1179175\Thermal=0.1228005\Dipole=0.2835475,-0.7347289,0.0013398\PG=C01 [X(C4H8O1)]\\@

THF-BF_3

1\1\GINC-R380\Freq\RM062X\6-31+G(d,p)\C4H8B1F3O1\ROOT\12-May-2016\0\\# N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\THF-BF3.freq\\0,1\C,-1.5367935197,-1.2438918405,-0.2385456758\C,-2.959133266,-0.7136073906,-0.3137206693\C,-2.7911748562,0.7276440765,0.1790961576\C,-1.494991119,1.1493652796,-0.4943829962\O,-0.7107600846,-0.0840109616,-0.5739982872\H,-1.2879348114,-2.025145959,-0.9549968515\H,-1.261907195,-1.5562480739,0.7721112144\H,-3.6406232422,-1.3025068407,0.3027275862\H,-3.3224481931,-0.7285315945,-1.3460286215\H,-2.6706666848,0.7469336118,1.266238242\H,-3.6238863278,1.3776924585,-0.0955008447\H,-0.9024535997,1.8745872927,0.0621151408\H,-1.6393296291,1.4898411338,-1.5218590922\B,0.7263607888,-0.0384149389,0.178422614\F,0.3988851037,0.20052124,1.4947503033\F,1.2370860461,-1.2825731432,-0.0496355266\F,1.3742605899,0.99838565,-0.4246826936\\Version=ES64L-G09RevD.01\State=1-A\HF=-556.8587286\RMSD=2.627e-09\RMSF=9.094e-06\ZeroPoint=0.133727\Thermal=0.1423951\Dipole=-2.5898861,0.0028404,-0.4711048\PG=C01 [X(C4H8B1F3O1)]\\@

TMPy

1\1\GINC-R233\Freq\RM062X\6-31+G(d,p)\C8H11N1\ROOT\12-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\TMP.freq\\0,1\C,-4.0773556833,1.5132853924,-0.002635164\C,-3.8158148034,0.142841341,0.0063031635\N,-2.5701652815,-0.3488577882,0.0061229744\C,-1.5436282218,0.5065609774,-0.0029550829\C,-1.7253555594,1.8931132049,-0.0122422208\C,-3.0150815692,2.4189504587,-0.0121742302\C,-3.2651795464,3.9039629539,-0.0219577457\C,-4.928319605,-0.8709521768,0.0167558644\C,-0.1682405542,-0.1050346021,-0.0026675172\H,-5.1041344364,1.8697821245,-0.0021409156\H,-0.8622045702,2.5528489933,-0.0194536986\H,-2.3277191748,4.4643207741,-0.0286838096\H,-3.8382395289,4.2052880571,0.8600294961\H,-3.8434292198,4.1927874371,-0.9047395925\H,-5.9100159184,-0.3923565033,0.0162526586\H,-4.8444257322,-1.5074825647,0.9018664092\H,-4.8496060838,-1.5199606889,-0.859726837\H,-0.0454881809,-0.7468380387,-0.8793902787\H,-0.0403074792,-0.7343590715,0.8823219954\H,0.6127596302,0.6583495138,-0.0103715984\\Version=ES64L-G09RevD.01\State=1-A'\HF=-366.0915237\RMSD=5.152e-09\RMSF=7.379e-05\ZeroPoint=0.1722272\Thermal=0.1818326\Dipole=-0.1415701,0.7768519,-0.0050865\PG=CS [SG(C8H5N1),X(H6)]\\@

TMPy-BF_3

1\1\GINC-R39\Freq\RM062X\6-31+G(d,p)\C8H11B1F3N1\ROOT\13-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\TMP-BF3.freq\\0,1\C,-4.0463584492,1.5239337821,0.0193571057\C,-3.7642294834,0.1637223699,-0.0347893364\N,-2.477041337,-0.2769030507,-0.0400597223\C,-1.4581324687,0.6203265197,-0.0548579061\C,-1.7228822481,1.9860731603,0.0047673058\C,-3.0257754859,2.4680910201,0.0619660404\C,-3.3188521482,3.9377023368,0.1676963745\C,-4.9109517192,-0.8080405985,-0.1013910111\C,-0.023608857,0.1799131283,-0.1652703359\H,-5.0854721684,1.8365703415,0.0222067361\H,-0.8846729734,2.674692446,-0.0047487096\H,-2.5127233773,4.5346187397,-0.2637424324\H,-3.4202603208,4.220931017,1.2205247842\H,-4.2539186324,4.190576678,-0.3368344454\H,-5.8096939304,-0.2692759436,-0.4047248895\H,-5.080184068,-1.2661901414,0.8749198977\H,-4.7121312391,-1.6119386628,-0.8096632134\H,0.1147106887,-0.5105353165,-0.9979650113\H,0.303322459,-0.3396530415,0.7363724188\H,0.599926414,1.0613946575,-0.3192098908\B,-2.2483243976,-1.9402247404,-0.042153015\F,-2.6321504895,-2.347308385,-1.3047639607\F,-3.0664445942,-2.4179791113,0.9601177434\F,-0.928412174,-2.206827205,0.2223044731\\Version=ES64L-G09RevD.01\State=1-A\HF=-690.6019783\RMSD=4.194e-09\RMSF=2.640e-06\ZeroPoint=0.1888896\Thermal=0.2018102\Dipole=-0.4706168,3.1058146,0.0573481\PG=C01 [X(C8H11B1F3N1)]\\@

DMF

1\1\GINC-R210\Freq\RM062X\6-31+G(d,p)\C3H7N1O1\ROOT\12-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\DMF.CS.freq\\0,1\O,0.,-0.05319,-1.86115\C,0.,-0.62547,-0.78705\N,0.,-0.01823,0.42838\C,0.,-0.77195,1.66215\C,0.,1.42764,0.52591\H,0.,-1.72779,-0.70587\H,0.88954,-0.53926,2.25857\H,0.,-1.84125,1.43971\H,-0.88954,-0.53926,2.25857\H,-0.89044,1.77254,1.06328\H,0.,1.84005,-0.48265\H,0.89044,1.77254,1.06328\\Version=ES64L-G09RevD.01\State=1-A'\HF=-248.4089956\RMSD=2.121e-09\RMSF=9.600e-06\ZeroPoint=0.1034226\Thermal=0.1095336\Dipole=0.,-0.2199862,1.646725\PG=CS [SG(C3H3N1O1),X(H4)]\\@

DMF-BF_3

1\1\GINC-R408\Freq\RM062X\6-31+G(d,p)\C3H7B1F3N1O1\ROOT\12-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\DMF-BF3.freq\\0,1\O,-3.7906476665,2.1729228407,0.4373374347\C,-3.5381971521,0.9505266369,0.3016526823\N,-2.3254994297,0.4977493307,0.0550914758\C,-2.0651837137,-0.9264898083,-0.0967973622\C,-1.1883879707,1.4024036468,-0.0769220523\H,-4.3393060368,0.2113557265,0.3871755736\H,-1.6540938186,-1.1225206556,-1.0905845354\H,-2.9927278365,-1.4868055451,0.024144486\H,-1.3469771123,-1.2530899274,0.6598731204\H,-0.4405169604,1.1551147899,0.6810557146\H,-1.5290607023,2.4268336909,0.0592092908\H,-0.7477703969,1.2856995581,-1.0705153981\B,-5.3297849751,2.518900824,0.7328142881\F,-5.3655688631,3.8718360647,0.8421323681\F,-6.0087612693,2.0001502489,-0.3511663372\F,-5.6162360959,1.8291625782,1.8936192507\\Version=ES64L-G09RevD.01\State=1-A\HF=-572.9154384\RMSD=3.193e-09\RMSF=2.609e-05\ZeroPoint=0.1188932\Thermal=0.129148\Dipole=3.1730937,-2.4506292,-0.7392246\PG=C01 [X(C3H7B1F3N1O1)]\\@

Py

1\1\GINC-R115\Freq\RM062X\6-31+G(d,p)\C5H5N1\ROOT\11-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\Pyridine.freq\\0,1\N,0.,-1.3827862391,0.\C,1.1399435702,-0.6874573012,0.\C,1.1963677911,0.7057511185,0.\C,0.,1.41685283,0.\C,-1.1963677911,0.7057511185,0.\C,-1.1399435702,-0.6874573012,0.\H,2.0553325973,-1.274344197,0.\H,2.1547865551,1.2135691334,0.\H,0.,2.5025659017,0.\H,-2.1547865551,1.2135691334,0.\H,-2.0553325973,-1.274344197,0.\\Version=ES64L-G09RevD.01\State=1-A1\HF=-248.1861963\RMSD=1.115e-09\RMSF=3.681e-05\ZeroPoint=0.0895966\Thermal=0.0938629\Dipole=0.,0.9256751,0.\PG=C02V [C2(H1C1N1),SGV(C4H4)]\\@

Py-BF_3

1\1\GINC-R410\Freq\RM062X\6-31+G(d,p)\C5H5B1F3N1\ROOT\12-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\Pyridine-BF3.freq\\0,1\C,0.,-1.141019774,0.8445546714\C,0.,-1.1997054822,2.2288171201\C,0.,-0.0062614986,2.9488638122\C,0.,1.2043620427,2.263131345\C,0.,1.1868421565,0.874464066\N,0.,0.0331467715,0.1974985401\H,0.,-2.0228039091,0.2129944881\H,0.,-2.1616310081,2.7269003859\H,0.,-0.0215811655,4.0339288814\H,0.,2.1522459106,2.7875157905\H,0.,2.082567546,0.2640581935\B,0.,-0.006393008,-1.4603731849\F,0.,1.3126049057,-1.8511112832\F,-1.1460202021,-0.6929017439,-1.791431413\F,1.1460202021,-0.6929017439,-1.791431413\\Version=ES64L-G09RevD.01\State=1-A'\HF=-572.7017421\RMSD=4.257e-09\RMSF=5.736e-05\ZeroPoint=0.1050851\Thermal=0.1134106\Dipole=0.,0.0617528,3.2567381\PG=CS [SG(C5H5B1F1N1),X(F2)]\\@

TEA

1\1\GINC-R59\Freq\RM062X\6-31+G(d,p)\C6H15N1\ROOT\12-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\Triethylamine.freq\\0,1\N,0.0000001724,0.0000003448,0.0056694197\C,-1.3542914062,0.330342702,-0.4375259929\C,0.3910610885,-1.338021745,-0.4375259929\C,0.963230835,1.0076800775,-0.4375259929\C,-2.430562189,-0.316212352,0.4268450029\H,-1.4939279958,0.0537947042,-1.5009528429\H,-1.4742313546,1.4162972626,-0.3838957446\H,-0.4894331741,-1.9848700675,-0.3838957446\C,1.4891295815,-1.9468220572,0.4268450029\H,0.7003769747,-1.32067658,-1.5009528429\C,0.9414331247,2.2630354437,0.4268450029\H,0.7935515383,1.2668829102,-1.5009528429\H,1.963665046,0.5685738394,-0.3838957446\H,-2.3749516023,-1.4081006774,0.4049898379\H,-3.4258908086,-0.0286257751,0.0753547903\H,-2.316468097,0.0063696694,1.4649351504\H,1.1527183102,-2.0093046858,1.4649351504\H,2.4069273161,-1.3527177138,0.4049898379\H,1.73773661,-2.9525952153,0.0753547903\H,-0.0319751965,2.7608194256,0.4049898379\H,1.6881547158,2.9812220249,0.0753547903\H,1.163750304,2.0029360509,1.4649351504\\Version=ES64L-G09RevD.01\State=1-A\HF=-292.2780627\RMSD=4.181e-10\RMSF=1.743e-05\ZeroPoint=0.2073077\Thermal=0.2166872\Dipole=0.,0.,-0.2373411\PG=C03 [C3(N1),X(C6H15)]\\@

TEA-BF_3

1\1\GINC-R210\Freq\RM062X\6-31+G(d,p)\C6H15B1F3N1\ROOT\12-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\TEA-BF3.freq\\0,1\B,-1.0709151967,-2.1302253449,-1.9709976577\F,-0.3518625292,-2.8876302833,-1.0665208586\F,-2.2766141158,-2.7143456993,-2.308418702\F,-1.2155625812,-0.8179663783,-1.5637135543\N,-0.1592984115,-2.0878568276,-3.3782748204\C,0.8337755225,-0.9628535277,-3.3163964924\C,-1.0540066905,-1.8799571355,-4.5664414112\C,0.5838424095,-3.3814376149,-3.5510773971\H,0.2571575338,-0.0500181969,-3.1796981771\H,1.3302797112,-0.9207606588,-4.2947917318\C,1.8570170086,-1.0719359237,-2.1941435635\C,-1.8284913763,-0.5690214334,-4.5641378557\H,-1.7615931667,-2.7068716649,-4.5676463207\H,-0.4214140667,-1.958248593,-5.4604323908\H,1.2091637184,-3.4978252085,-2.6679753308\H,1.2339530107,-3.2618131112,-4.4277794186\C,-0.2987455658,-4.6137513687,-3.6953784066\H,1.3684665077,-1.2113382146,-1.2282667554\H,2.4207130955,-0.1361702351,-2.1610031123\H,2.5730165875,-1.8813464936,-2.3505004986\H,-2.3856201127,-0.4426971458,-3.6342759784\H,-2.5433383141,-0.599519869,-5.3903133012\H,-1.1879390555,0.302113884,-4.7159695076\H,-1.0128184826,-4.6849766564,-2.8731467118\H,0.3470140427,-5.4950054702,-3.6654740473\H,-0.842839483,-4.6371908286,-4.6417659982\\Version=ES64L-G09RevD.01\State=1-A\HF=-616.8030909\RMSD=4.403e-09\RMSF=1.825e-05\ZeroPoint=0.2250952\Thermal=0.2377715\Dipole=1.2482725,0.0579118,-1.9266136\PG=C01 [X(C6H15B1F3N1)]\\@

MAc

1\1\GINC-R38\Freq\RM062X\6-31+G(d,p)\C3H6O2\ROOT\13-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\MA.freq\\0,1\O,0.,1.32551,0.32755\C,0.,0.12553,0.46119\C,0.,-0.61188,1.77236\O,0.,-0.72764,-0.57964\C,0.,-0.11516,-1.87083\H,0.,0.10718,2.5892\H,0.88187,-1.25377,1.83293\H,-0.88187,-1.25377,1.83293\H,0.,-0.93547,-2.5861\H,0.88897,0.50668,-1.9949\H,-0.88897,0.50668,-1.9949\\Version=ES64L-G09RevD.01\State=1-A'\HF=-268.2835315\RMSD=9.420e-10\RMSF=3.411e-05\ZeroPoint=0.0908387\Thermal=0.0969473\Dipole=0.,-0.7272354,-0.150178\PG=CS [SG(C3H2O2),X(H4)]\\@

MAc-BF_3

1\1\GINC-R517\Freq\RM062X\6-31+G(d,p)\C3H6B1F3O2\ROOT\15-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test Genchk RM062X/6-31+G(d,p) Freq\\MA-BF3.CS.freq\\0,1\O,0.,-0.4740557666,-0.2721789614\C,0.,0.4377119475,-1.1162999634\C,0.,1.8946671213,-0.8102289058\O,0.,0.1304669532,-2.3853271123\C,0.,-1.272133374,-2.7258585191\H,0.8779647248,2.1181736959,-0.199432676\H,-0.8779647248,2.1181736959,-0.199432676\H,0.,2.4724020329,-1.7317549793\H,0.,-1.2975185177,-3.8122378569\H,-0.8921112545,-1.7474133946,-2.3174851415\H,0.8921112545,-1.7474133946,-2.3174851415\B,0.,-0.1913531269,1.3430891591\F,-1.1471473685,0.5331851415,1.5537283655\F,1.1471473685,0.5331851415,1.5537283655\F,0.,-1.4392781552,1.869216043\\Version=ES64L-G09RevD.01\State=1-A'\HF=-592.7813792\RMSD=1.742e-09\RMSF=2.285e-05\ZeroPoint=0.1059951\Thermal=0.1159622\Dipole=0.,0.3707695,-2.7188058\PG=CS [SG(C3H2B1F1O2),X(H4F2)]\\@

PC

1\1\GINC-R60\Freq\RM062X\6-31+G(d,p)\C4H6O3\ROOT\13-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\PC.freq\\0,1\O,0.5555076856,-0.2730068939,1.6136768192\C,0.945056933,-0.4393031038,0.2427549591\C,2.2783072933,0.3112881765,0.2070693034\O,2.7093899173,0.2646072122,1.5655306343\C,1.6407225348,0.0261503022,2.3651457047\O,1.6577960377,0.0739514262,3.5544047382\C,-0.125014819,0.1075749309,-0.6728272193\H,1.0982481298,-1.5117639261,0.0736698992\H,2.1475137318,1.3580077972,-0.0903189235\H,3.0339457419,-0.1636572517,-0.4186076657\H,-0.3060152977,1.162985127,-0.4528338374\H,-1.0586170922,-0.442974305,-0.5430272937\H,0.1918192038,0.0118605083,-1.7156571185\\Version=ES64L-G09RevD.01\State=1-A\HF=-381.582412\RMSD=1.988e-09\RMSF=1.997e-05\ZeroPoint=0.1042297\Thermal=0.1103965\Dipole=-0.1622192,-0.0919574,-2.2999153\PG=C01 [X(C4H6O3)]\\@

PC-BF_3

1\1\GINC-R38\Freq\RM062X\6-31+G(d,p)\C4H6B1F3O3\ROOT\15-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\PC-BF3.2.freq\\0,1\O,-0.020146341,-0.0526176097,0.0099640463\C,-0.0090304914,-0.0179026646,1.4595235892\C,1.4959361152,0.0102377752,1.7511789441\O,2.0581022781,0.4797044483,0.5124399169\C,1.1538801897,0.3271951691,-0.44184261\O,1.4216619161,0.5274380161,-1.6185970316\C,-0.7540437606,-1.2127195934,2.0024355731\H,-0.489667861,0.9222255479,1.7464004265\H,1.8999249267,-0.9860537629,1.9527596878\H,1.7820029196,0.7047681598,2.5392777591\H,-0.298672915,-2.1393088699,1.6442308215\H,-1.7972515982,-1.1859660692,1.6838884032\H,-0.7230031532,-1.199151422,3.0955960374\B,0.2189820009,0.4153892169,-2.8097124843\F,-0.185467873,-0.8829371759,-2.715205712\F,-0.7021390727,1.3325945572,-2.3952802162\F,0.9083043614,0.7377862706,-3.9261410824\\Version=ES64L-G09RevD.01\State=1-A\HF=-706.0725934\RMSD=2.762e-09\RMSF=2.757e-05\ZeroPoint=0.1186823\Thermal=0.1292914\Dipole=0.2153788,-0.543943,4.1517032\PG=C01 [X(C4H6B1F3O3)]\\@

NM

1\1\GINC-R38\Freq\RM062X\6-31+G(d,p)\C1H3N1O2\ROOT\13-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\NM.freq\\0,1\C,0.,-0.3470678598,1.3854269713\N,0.,0.0108360922,-0.0631062871\H,0.8909235569,0.1025717526,1.8212163321\H,0.,-1.4298138246,1.4670705258\H,-0.8909235569,0.1025717526,1.8212163321\O,0.,-0.8968719179,-0.8716390628\O,0.,1.1976240048,-0.3306348113\\Version=ES64L-G09RevD.01\State=1-A'\HF=-244.9144474\RMSD=2.618e-09\RMSF=1.664e-04\ZeroPoint=0.050789\Thermal=0.0551036\Dipole=0.,-0.3690886,1.4800496\PG=CS [SG(C1H1N1O2),X(H2)]\\@

NM-BF_3

1\1\GINC-R37\Freq\RM062X\6-31+G(d,p)\C1H3B1F3N1O2\ROOT\15-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\NM-BF3.freq\\0,1\B,0.,-0.026301174,1.1733179076\O,0.,0.7829248142,-0.4560769574\N,0.,0.06163028,-1.4714154816\O,0.,-1.1339810212,-1.4663550591\C,0.,0.8051566251,-2.7585703209\F,0.,1.0899052177,1.9215654639\F,1.1506709003,-0.7258654668,1.112655897\F,-1.150670903,-0.7258654668,1.112655897\H,-0.8928823754,1.4290149029,-2.7598405175\H,0.8928823754,1.4290149029,-2.7598405175\H,0.,0.0698063878,-3.5574363054\\Version=ES64L-G09RevD.01\State=1-A'\HF=-569.3969645\RMSD=1.633e-09\RMSF=4.026e-05\ZeroPoint=0.0649427\Thermal=0.0736442\Dipole=0.,0.8209009,-2.8319386\PG=CS [SG(C1H1B1F1N1O2),X(H2F2)]\\@

DMSO

1\1\GINC-R66\Freq\RM062X\6-31+G(d,p)\C2H6O1S1\ROOT\18-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\DMSO.freq\\0,1\C,-0.3160054258,0.8140175039,-1.3516833052\S,0.3891643749,-0.1700500565,0.\C,-0.3160054258,0.8140175039,1.3516833052\O,-0.3590029273,-1.4806071734,0.\H,0.0888411937,1.8284560906,-1.3282896733\H,-1.4036587275,0.8168048351,-1.2482134216\H,-0.0364677642,0.3211201853,-2.2835481051\H,0.0888411937,1.8284560906,1.3282896733\H,-0.0364677642,0.3211201853,2.2835481051\H,-1.4036587275,0.8168048351,1.2482134216\\Version=ES64L-G09RevD.01\State=1-A'\HF=-553.0828047\RMSD=2.895e-09\RMSF=2.025e-05\ZeroPoint=0.0802047\Thermal=0.0857895\Dipole=0.1774553,1.7597685,0.\PG=CS [SG(O1S1),X(C2H6)]\\@

DMSO-BF_3

1\1\GINC-R48\Freq\RM062X\6-31+G(d,p)\C2H6B1F3O1S1\ROOT\18-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\DMSO-BF3.freq\\0,1\C,-0.1649282791,0.8024101363,-1.232299252\S,0.5531171395,0.0633402134,0.2413044526\C,-0.480316996,0.8068574005,1.5049608452\O,-0.0407609382,-1.3909558281,0.2315420727\H,0.078391445,1.8668779109,-1.249947035\H,-1.2429937769,0.6329383724,-1.2207360353\H,0.2975973621,0.284636341,-2.0736141966\H,-0.3048321612,1.8842840481,1.5142723632\H,-0.1845468896,0.3666024764,2.4573649957\H,-1.5224515096,0.5707074098,1.2838354113\B,0.95959035,-2.4405549,-0.4028050185\F,0.2154383666,-3.5613491925,-0.598124254\F,1.388066585,-1.8255242425,-1.5856902521\F,1.9997793023,-2.5777701457,0.4882059029\\Version=ES64L-G09RevD.01\State=1-A\HF=-877.5959108\RMSD=1.471e-09\RMSF=6.112e-06\ZeroPoint=0.0951652\Thermal=0.104803\Dipole=-1.2290612,3.699625,0.6855658\PG=C01 [X(C2H6B1F3O1S1)]\\@

TMU

1\1\GINC-R48\Freq\RM062X\6-31+G(d,p)\C5H12N2O1\ROOT\18-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\TMU.C2.freq\\0,1\C,0.,0.51049,0.\O,0.,1.73495,0.\N,-0.11176,-0.22744,1.16939\C,-0.34822,0.54361,2.37832\C,0.67462,-1.43504,1.37793\N,0.11176,-0.22744,-1.16939\C,-0.67462,-1.43504,-1.37793\C,0.34822,0.54361,-2.37832\H,-1.05856,1.34198,2.16916\H,0.57796,0.99643,2.75812\H,-0.75891,-0.12298,3.14165\H,1.08782,-1.79186,0.43535\H,0.06032,-2.22632,1.8223\H,1.5115,-1.22538,2.05798\H,-1.08782,-1.79186,-0.43535\H,-0.06032,-2.22632,-1.8223\H,-1.5115,-1.22538,-2.05798\H,1.05856,1.34198,-2.16916\H,-0.57796,0.99643,-2.75812\H,0.75891,-0.12298,-3.14165\\Version=ES64L-G09RevD.01\State=1-A\HF=-382.3354627\RMSD=1.371e-09\RMSF=1.052e-05\ZeroPoint=0.1777616\Thermal=0.1877879\Dipole=0.,-1.3802493,0.\PG=C02 [C2(C1O1),X(C4H12N2)]\\@

TMU-BF_3

1\1\GINC-R150\Freq\RM062X\6-31+G(d,p)\C5H12B1F3N2O1\ROOT\18-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\TMU-BF3.freq\\0,1\C,-1.22010288,0.4217014103,2.1374836211\O,-1.8010222479,-0.5161682816,2.7827886715\N,-1.1783082795,1.6832474997,2.6045172388\C,-1.5509443248,1.9461980966,3.993620699\C,-1.268298731,2.8371965775,1.7172435987\N,-0.6037276372,0.1018960849,0.984593545\C,0.5599646731,0.8119410344,0.4754377563\C,-0.8924331078,-1.1871897258,0.3612034982\H,-1.352231023,1.0660913803,4.6026839731\H,-2.6153845665,2.186901053,4.066572643\H,-0.9492054282,2.7867103954,4.3487826049\H,-1.3381339946,2.5156968097,0.6790856776\H,-0.4071865843,3.5018174142,1.8410118575\H,-2.1827748071,3.3855257379,1.9645836056\H,0.9135132352,1.5324965135,1.2126392412\H,0.3375953495,1.3299465502,-0.4633136283\H,1.3558713545,0.0837721132,0.2906713856\H,-1.8746713234,-1.5356815865,0.6752298138\H,-0.1409054409,-1.9300741841,0.6492907988\H,-0.874371259,-1.0570672495,-0.7236853999\B,-3.3222291012,-0.44345661,3.189131447\F,-3.8182293459,0.7092854196,2.5826548115\F,-3.3740066989,-0.379554902,4.5606753669\F,-3.8671878308,-1.5880115509,2.6660271731\\Version=ES64L-G09RevD.01\State=1-A\HF=-706.8461721\RMSD=3.771e-09\RMSF=1.718e-05\ZeroPoint=0.1934455\Thermal=0.207275\Dipole=2.8563926,1.7422008,-1.7373054\PG=C01 [X(C5H12B1F3N2O1)]\\@

ISO

1\1\GINC-R113\Freq\RM062X\6-31+G(d,p)\C9H14O1\ROOT\18-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\VAL.freq\\0,1\C,-2.9385104244,1.8478676227,0.2063869559\C,-2.9682172379,0.528123453,-0.0442972408\C,-1.7145108812,-0.2430867203,-0.3799359475\C,-0.4107666675,0.4264835924,0.085866021\C,-0.4494292091,1.9032947242,-0.3350605 56\C,-1.6851631934,2.6292466842,0.1643111641\C,-4.243968837,-0.2612341477,-0.0215603136\C,-0.2759735916,0.3219610373,1.6114368547\C,0.783906899,-0.2683979012,-0.5708064707\O,-1.6560517131,3.8051961513,0.4801335307\H,-3.8391715382,2.4018662807,0.4582872582\H,-1.6869953841,-0.3815807068,-1.4724230162\H,-1.7863878694,-1.252941951,0.0472730184\H,-0.4650108378,1.9687022017,-1.4333994804\H,0.433464389,2.4480255829,0.0140781118\H,-4.2064308218,-1.0180525472,0.7704530965\H,-4.3760894596,-0.7986596707,-0.9677861048\H,-5.1138434482,0.3772956439,0.1437525034\H,-1.1216962721,0.7851621613,2.1289914414\H,0.6384817738,0.8213170506,1.9480517395\H,-0.2213441651,-0.7275690762,1.920407512\H,0.7340531548,-0.1942611355,-1.6625628212\H,0.8109185309,-1.3305700679,-0.3024126048\H,1.7246568038,0.1859317383,-0.2422446517\\Version=ES64L-G09RevD.01\State=1-A\HF=-426.4420237\RMSD=1.750e-09\RMSF=1.509e-05\ZeroPoint=0.212312\Thermal=0.2226768\Dipole=-0.1051989,-1.6843748,-0.3771675\PG=C01 [X(C9H14O1)]\\@

ISO-BF_3

1\1\GINC-R116\Freq\RM062X\6-31+G(d,p)\C9H14B1F3O1\ROOT\18-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\VAL-BF3.2.freq\\0,1\C,-3.0964856154,1.7655935461,0.1474669108\C,-3.0405163752,0.4438936462,-0.1204813747\C,-1.7353405306,-0.2452510715,-0.4139840945\C,-0.5005054213,0.4778590379,0.1445757512\C,-0.5858948209,1.9650200735,-0.2331603048\C,-1.8992498815,2.5821617094,0.1471273632\C,-4.272734775,-0.403444991,-0.1576648962\C,-0.4383545712,0.3314313407,1.6717443896\C,0.7666498794,-0.1215620231,-0.4686982981\O,-2.0302783376,3.793548688,0.4244473695\H,-4.0317385201,2.2733514259,0.3620136633\H,-1.6521760171,-0.3313798087,-1.5093594546\H,-1.7761183048,-1.2744787928,-0.0341061502\H,-0.5093660177,2.0899424953,-1.324631165\H,0.2330264916,2.539686953,0.204156477\H,-4.2283725282,-1.1530375932,0.640748895\H,-4.3222306465,-0.9532002862,-1.1041595863\H,-5.1825250572,0.1869007471,-0.0398708371\H,-1.3347059253,0.7237160918,2.1625850834\H,0.4230867086,0.8758711938,2.0701496725\H,-0.3334573077,-0.7226599861,1.9491032996\H,0.76832446,-0.0193082091,-1.5590017968\H,0.8452935011,-1.1864071314,-0.2247067349\H,1.6577202275,0.3804678284,-0.0790925303\B,-0.8131718819,4.8493991746,0.4477893453\F,-0.2368287881,4.7449205503,-0.7998643351\F,0.0151580248,4.4095655456,1.4581438784\F,-1.4216079695,6.0379898455,0.6932594598\\Version=ES64L-G09RevD.01\State=1-A\HF=-750.9457307\RMSD=2.936e-09\RMSF=7.977e-06\ZeroPoint=0.2272385\Thermal=0.2417147\Dipole=-1.1242284,-3.878409,-0.5629796\PG=C01 [X(C9H14B1F3O1)]\\@

9.2 Benchmarking: Addition rate coefficients

nBA

1\1\GINC-R2428\Freq\RM062X\6-31+G(d,p)\C7H12O2\ROOT\24-Jul-2014\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\BA_mon.freq\\0,1\C,-0.0188428796,0.,0.0176577376\C,0.2637326868,0.,1.4782603662\C,0.9863249622,0.,-0.8550546549\H,-1.0617363075,0.,-0.2818224162\H,0.8081405903,0.,-1.9248048797\H,2.0131372006,0.,-0.5004516833\O,-0.8741184201,0.,2.1918234602\O,1.3655939966,0.,1.9780727574\C,-0.7159602625,0.,3.6178367404\C,-2.0983880318,0.,4.2378156641\H,-0.1387119519,-0.8843470923,3.9088391019\H,-0.1387119519,0.8843470923,3.9088391019\C,-2.0337666902,0.,5.7647654041\H,-2.6486925949,0.8813379203,3.8866594975\H,-2.6486925949,-0.8813379203,3.8866594975\C,-3.42212054,0.,6.4011522559\H,-1.4720841324,-0.8786600534,6.1058916738\H,-1.4720841324,0.8786600534,6.1058916738\H,-3.3613618768,0.,7.4926026628\H,-3.9908587737,0.884045505,6.0956044406\H,-3.9908587737,-0.884045505,6.0956044406\\Version=ES64L-G09RevD.01\State=1-A'\HF=-424.2401244\RMSD=1.966e-09\RMSF=3.127e-05\ZeroPoint=0.1822958\Thermal=0.1928573\Dipole=-0.6796645,0.,-0.0685666\PG=CS [SG(C7H4O2),X(H8)]\\@

tBA

1\1\GINC-R46\Freq\RM062X\6-31+G(d,p)\C7H12O2\ROOT\11-Mar-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\TBA.scis.freq\\0,1\C,0.,0.776025822,2.1934188427\C,0.,0.2218483612,3.4036971867\C,0.,-0.0877936611,0.9780937224\O,0.,-1.2985535627,0.9989585257\O,0.,0.6659930335,-0.1307099496\C,0.,0.0553227909,-1.4565067818\H,0.,0.8258433709,4.3044676037\H,0.,-0.859795316,3.504448198\C,0.,1.2630247435,-2.3867834626\C,-1.2676630271,-0.7732015319,-1.6516919385\C,1.2676630271,-0.7732015319,-1.6516919385\H,-0.8881014036,1.8770297386,-2.2136553787\H,0.,0.9307027601,-3.4285728731\H,0.8881014036,1.8770297386,-2.2136553787\H,-2.1504932393,-0.1645376922,-1.4335864406\H,-1.2708401034,-1.6534099461,-1.0080710015\H,-1.3250271033,-1.0975546893,-2.6952907212\H,2.1504932393,-0.1645376922,-1.4335864406\H,1.3250271033,-1.0975546893,-2.6952907212\H,1.2708401034,-1.6534099461,-1.0080710015\H,0.,1.8493198931,2.0349199593\\Version=ES64L-G09RevD.01\State=1-A'\HF=-424.2485877\RMSD=2.951e-09\RMSF=8.621e-05\ZeroPoint=0.1809139\Thermal=0.1912886\Dipole=0.,0.5737296,-0.2166445\\PG=CS [SG(C5H4O2),X(C2H8)]\\@

tBMA

1\1\GINC-R59\Freq\RM062X\6-31+G(d,p)\C8H14O2\ROOT\11-Mar-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\TBMA.strans.freq\\0,1\C,0.,-0.3674120715,2.0518842867\C,0.,-1.6990220842,2.1502532377\C,0.,0.5697868222,3.2251935323\C,0.,0.3100153823,0.7136702397\O,0.,1.5174913676,0.6021398774\O,0.,-0.5508012188,-0.3118870997\C,0.,-0.0772537933,-1.6921856666\H,0.,-2.1818358483,3.1231129538\H,0.,-2.3282334039,1.267764269\H,0.,0.0109213611,4.162865123\H,-0.8769190713,1.2226789167,3.1963305247\H,0.8769190713,1.2226789167,3.1963305247\C,0.,-1.3744456533,-2.4934326156\C,1.2678365196,0.7259497864,-1.9723863178\C,-1.2678365196,0.7259497864,-1.9723863178\H,0.8883589211,-1.9673463536,-2.2584808882\H,0.,-1.151499965,-3.5639071574\H,-0.8883589211,-1.9673463536,-2.2584808882\H,2.1503894014,0.1438417333,-1.6900316914\H,1.2705453579,1.6695349756,-1.4259995399\H,1.3265059518,0.9380654903,-3.0443275784\H,-2.1503894014,0.1438417333,-1.6900316914\H,-1.3265059518,0.9380654903,-3.0443275784\H,-1.2705453579,1.6695349756,-1.4259995399\\Version=ES64L-G09RevD.01\State=1-A'\HF=-463.5493921\RMSD=3.761e-09\RMSF=2.482e-05\ZeroPoint=0.209045\Thermal=0.2209123\Dipole=0.,-0.6557418,-0.234147\\PG=CS [SG(C6H4O2),X(C2H10)]\\@

MMA

1\1\GINC-V1373\Freq\RM062X\6-31+G(d,p)\C5H8O2\BXN501\10-Jul-2012\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\MMA.a.M062X.freq\\0,1\C,-0.0404335614,0.,-0.123106065\O,0.0337832672,0.,1.3028467532\C,1.2783193205,0.,1.8088113138\O,2.2702054537,0.,1.1141723696\C,1.3229287015,0.,3.3033846124\C,0.1971402252,0.,4.0211239225\H,-0.7762970054,0.,3.544306561\H,0.232742561,0.,5.1065256993\C,2.7058582071,0.,3.8876343073\H,2.6614244396,0.,4.9782753493\H,3.2657787588,-0.8772332683,3.5515045882\H,3.2657787588,0.8772332683,3.5515045882\H,-1.1021744109,0.,-0.362853584\H,0.4475571379,-0.8890227765,-0.5279907051\H,0.4475571379,0.8890227765,-0.5279907051\\Version=EM64L-G09RevA.02\State=1-A'\HF=-345.6504672\RMSD=6.061e-09\RMSF=7.295e-05\ZeroPoint=0.1247988\Thermal=0.1327678\Dipole=-0.6480922,0.,0.2436116\PG=CS [SG(C5H4O2),X(H4)]\\@

Benzyl rad

1\1\GINC-R68\Freq\UM062X\6-31+G(d,p)\C7H7(2)\ROOT\11-Mar-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/6-31+G(d,p) Freq\\benzyl_rad.C2V.freq\\0,2\C,0.0000026686,0.,0.0233241699\C,0.0000028485,0.,1.4356891485\C,1.214383052,0.,2.1716859761\C,1.2092937948,0.,3.556917597\C,0.0000032083,0.,4.260746761\C,-1.2092875575,0.,3.556917905\C,-1.2143771676,0.,2.1716862855\H,0.9291445844,0.,-0.5334717232\H,-0.9291393891,0.,-0.5334714865\H,2.1558111488,0.,1.6290511468\H,2.1502097182,0.,4.0985458318\H,0.0000033465,0.,5.345744547\H,-2.1502033429,0.,4.0985463795\H,-2.1558054026,0.,1.6290516959\\Version=ES64L-G09RevD.01\State=2-B1\HF=-270.7980298\S2=0.777328\S2-1=0.\S2A=0.750448\RMSD=1.155e-09\RMSF=1.462e-05\ZeroPoint=0.1154146\Thermal=0.1210963\Dipole=0.,0.,-0.0034716\PG=C02V [C2(H1C1C1C1),SGV(C4H6)]\\@

Cumyl rad

1\1\GINC-R37\Freq\UM062X\6-31+G(d,p)\C9H11(2)\ROOT\24-Feb-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/6-31+G(d,p) Freq\\cumyl_rad.C2V.freq\\0,2\C,0.,0.,1.67198\C,0.,0.,0.24082\C,0.,-1.20987,-0.50158\C,0.,-1.20471,-1.88873\C,0.,0.,-2.59642\C,0.,1.20471,-1.88873\C,0.,1.20987,-0.50158\C,0.,-1.29505,2.42721\C,0.,1.29505,2.42721\H,0.,-2.16059,0.0212\H,0.,-2.14837,-2.42612\H,0.,0.,-3.68142\H,0.,2.14837,-2.42612\H,0.,2.16059,0.0212\H,0.,-1.123,3.50514\H,0.88031,-1.90641,2.18697\H,-0.88031,-1.90641,2.18697\H,0.,1.123,3.50514\H,-0.88031,1.90641,2.18697\H,0.88031,1.90641,2.18697\\Version=ES64L-G09RevD.01\State=2-B1\HF=-349.3967524\S2=0.771086\S2-1=0.\S2A=0.750282\RMSD=6.895e-10\RMSF=1.188e-05\ZeroPoint=0.1722466\Thermal=0.1811014\Dipole=0.,0.,0.3489608\PG=C02V [C2(C1C1C1H1),SGV(C6H6),X(H4)]\\@

B rad

1\1\GINC-R1962\Freq\UM062X\6-31+G(d,p)\C7H5O1(2)\ROOT\30-Jun-2014\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/6-31+G(d,p) Freq\\B_rad.freq\\0,2\C,-5.7099596575,6.9308076636,0.0382980987\C,-5.715379641,6.6866890985,-1.3376491952\C,-4.9384062644,5.6631978507,-1.8790265612\C,-4.1502147029,4.8773700131,-1.0420021877\C,-4.1457823661,5.1222406095,0.331618709\C,-4.9252883183,6.1497528962,0.8785218354\H,-6.3179658807,7.7296593783,0.4506170902\H,-6.329881398,7.299397392,-1.9899515734\H,-4.9476195182,5.4794541537,-2.9482354716\H,-3.5357614626,4.0739626741,-1.437194775\C,-3.2996171501,4.2755937099,1.2136289536\H,-4.9037110806,6.3193304319,1.950760916\O,-3.1773529401,4.3442838088,2.3900342193\\Version=ES64L-G09RevD.01\State=2-A'\HF=-344.787223\S2=0.753726\S2-1=0.\S2A=0.750009\RMSD=2.352e-09\RMSF=1.114e-04\ZeroPoint=0.0983542\Thermal=0.1046996\Dipole=-0.7107667,0.6608125,-1.0174091\PG=CS [SG(C7H5O1)]\\@

T rad

1\1\GINC-R1179\Freq\UM062X\6-31+G(d,p)\C8H7O1S1(2)\ROOT\15-Feb-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/6-31+G(d,p) Freq\\T_rad.1.freq\\0,2\O,-0.1128200897,-0.0001309203,-0.000335855\C,-0.0146555899,0.0000238345,1.1818761788\C,1.2212966926,0.0000295183,1.9952739632\C,1.1267839526,0.0002295613,3.3851191369\C,2.275728737,0.0002389929,4.1712998272\C,3.5355559396,0.0000462034,3.5620873482\C,3.6278659686,-0.0001557667,2.1569081255\C,2.4838264516,-0.0001642825,1.3804250416\H,0.1440340562,0.0003781951,3.8476351327\H,2.1782810473,0.0003963696,5.2502820613\H,4.6064688301,-0.0003053017,1.6852738595\H,2.5477531594,-0.0003194449,0.2965369992\S,5.0641941837,0.0000356448,4.4407148199\C,4.5356797052,0.0003198766,6.1691665787\H,5.4543550732,0.0003218352,6.7573466372\H,3.9626593159,0.8977269508,6.4104754282\H,3.9625045018,-0.8969216546,6.4107232076\\Version=ES64L-G09RevD.01\State=2-A'\HF=-782.238338\S2=0.753875\S2-1=0.\S2A=0.75001\RMSD=2.328e-09\RMSF=2.615e-05\ZeroPoint=0.1275708\Thermal=0.137082\Dipole=0.8370128,0.000142,1.5516457\PG=CS [SG(C8H5O1S1),X(H2)]\\@

M rad

1\1\GINC-R99\Freq\UM062X\6-31+G(d,p)\C7H14N1O1(2)\ROOT\16-Feb-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/6-31+G(d,p) Freq\\M_rad.freq\\0,2\C,0.0989343365,-1.2836989388,2.4704186933\C,-0.1545180055,0.,1.7351056527\C,0.0989343365,1.2836989388,2.4704186933\N,0.1054157035,0.,0.3525352348\C,-0.2840565265,-1.2005809574,-0.3847642822\C,-0.2840565265,1.2005809574,-0.3847642822\C,0.266096371,-1.1578949812,-1.8022250723\O,-0.1610378868,0.,-2.4897391045\C,0.266096371,1.1578949812,-1.8022250723\H,-0.0600870935,-1.1321544709,3.5398364265\H,1.1354900288,-1.6394198892,2.3364526063\H,-0.5657282312,-2.0959527357,2.1589839149\H,1.1354900288,1.6394198892,2.3364526063\H,-0.0600870935,1.1321544709,3.5398364265\H,-0.5657282312,2.0959527357,2.1589839149\H,-1.3849308965,-1.2900390141,-0.4182956725\H,0.1180469171,-2.0837849493,0.1151807308\H,0.1180469171,2.0837849493,0.1151807308\H,-1.3849308965,1.2900390141,-0.4182956725\H,-0.0944877541,-2.0162215587,-2.3738673018\H,1.3669379428,-1.1852853562,-1.7699009346\H,1.3669379428,1.1852853562,-1.7699009346\H,-0.0944877541,2.0162215587,-2.3738673018\\Version=ES64L-G09RevD.01\State=2-A'\HF=-404.9143146\S2=0.753945\S2-1=0.\S2A=0.750012\RMSD=2.009e-09\RMSF=5.421e-06\ZeroPoint=0.2079459\Thermal=0.2174217\Dipole=0.22907,0.,0.3513634\PG=CS [SG(C1N1O1),X(C6H14)]\\@

Benzyl rad-MMA TS

1\1\GINC-R46\Freq\UM062X\6-31+G(d,p)\C12H15O2(2)\ROOT\11-Mar-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/6-31+G(d,p) Freq\\benzyl_MMA_TS.3.freq\\0,2\C,-0.042697066,0.0224301842,0.0539292839\C,-0.0324478619,-0.0087027827,1.4888185436\C,1.1786492459,-0.0017199939,2.211753344\C,1.1786371723,0.0514428786,3.5986086071\C,-0.02845989,0.1067938232,4.3015372639\C,-1.2371014272,0.107037079,3.6017228979\C,-1.2409660229,0.0486760262,2.2138179052\H,0.8832235425,-0.151069067,-0.4861965044\H,-0.9601618954,-0.2232730687,-0.4709854534\H,2.1193130525,-0.035774353,1.6676981406\H,2.1208025296,0.0503205402,4.1384351118\H,-0.0262466252,0.1516508353,5.3861201134\H,-2.1782081819,0.1599729087,4.1405285462\H,-2.1838531399,0.0569522006,1.6719592452\C,-0.1528329818,2.2251147241,-0.426846274\H,-0.1394304328,2.0030442784,-1.4904165716\H,0.8013774367,2.3921186823,0.0604345114\C,-1.3027666311,2.6825290162,0.149197758\C,-1.3137353847,3.1554697802,1.5491219231\O,-2.3165644694,3.5282123904,2.1270542753\O,-0.0985689211,3.1435727424,2.1312676569\C,-0.0737056143,3.5725161344,3.4905215932\C,-2.6421396282,2.6236074713,-0.52000721\H,0.9485310549,3.4121624174,3.8305353819\H,-0.7723603925,2.9805726146,4.0855015533\H,-0.3461881284,4.6287486386,3.5599195188\H,-3.3088404744,1.927242519,0.0030341732\H,-2.5426034086,2.3034391199,-1.5596546657\H,-3.1368746767,3.5988913893,-0.491353892\\Version=ES64L-G09RevD.01\State=2-A\HF=-616.4457758\S2=0.784266\S2-1=0.\S2A=0.750742\RMSD=2.554e-09\RMSF=3.690e-06\ZeroPoint=0.2417596\Thermal=0.2560365\Dipole=0.775873,-0.4394676,-0.2962825\PG=C01 [X(C12H15O2)]\\@

Cumyl rad-MMA TS

1\1\GINC-R2733\Freq\UM062X\6-31+G(d,p)\C14H19O2(2)\ROOT\29-Feb-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/6-31+G(d,p) Freq\\cumyl_MMA_TS.3.freq\\0,2\C,-0.7341319681,0.588482622,0.868253606\C,-1.9270278577,-0.1624651293,0.4801387575\C,-3.0676331048,0.483352479,-0.0382023556\C,-4.1747616616,-0.2399580175,-0.4665264132\C,-4.1799961727,-1.6330187805,-0.3954837953\C,-3.0619485043,-2.2925558759,0.1149421867\C,-1.9558942431,-1.5708628251,0.5488636588\C,-0.8190063889,2.0907243059,0.9365673029\C,0.2174974944,-0.0313358046,1.856972476\H,-3.0954700375,1.5656347015,-0.1043182416\H,-5.0402342412,0.2879029831,-0.8560392565\H,-5.0435421362,-2.1972589564,-0.7336585722\H,-3.0456402772,-3.3769245726,0.1693070935\H,-1.0981071269,-2.1157134092,0.9291141465\H,0.1670180363,2.5226706537,1.1287388723\H,-1.4820582435,2.4035611914,1.7561453918\H,-1.2045667305,2.5351477067,0.0147816356\H,1.127646356,0.5693622177,1.9460868705\H,0.5149496257,-1.0451304539,1.5822247883\H,-0.2481604346,-0.0813010615,2.8517608972\C,0.4682218238,0.4233749024,-0.9989624659\H,1.260093447,1.0084660347,-0.5366053433\H,-0.2982405593,0.9659882792,-1.5420963546\C,0.6961022351,-0.8941734624,-1.2905655292\C,-0.263182775,-1.6662226083,-2.1047920746\O,-0.1400910973,-2.8519348673,-2.3483944842\O,-1.2926247412,-0.9311406509,-2.5717843745\C,-2.2456477327,-1.6503246045,-3.3498726241\C,1.8612938822,-1.6767535977,-0.7629697775\H,-3.0508850894,-0.9456083742,-3.5534103113\H,-2.6211683438,-2.5084700682,-2.7886460184\H,-1.7898356889,-2.0002444453,-4.2798122125\H,1.5256303161,-2.5251923939,-0.1547875896\H,2.5140740888,-1.0418997942,-0.1590851791\H,2.4439678508,-2.1060783243,-1.58471471\\Version=ES64L-G09RevD.01\State=2-A\HF=-695.045669\S2=0.779755\S2-1=0.\S2A=0.750473\RMSD=3.468e-09\RMSF=3.096e-06\ZeroPoint=0.2988096\Thermal=0.3158655\Dipole=-0.2469745,0.989179,0.4990563\PG=C01 [X(C14H19O2)]\\@

B rad-nBA TS

1\1\GINC-R248\Freq\UM062X\6-31+G(d,p)\C14H17O3(2)\ROOT\30-Jul-2014\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=671088640\\B_BA_TS.1.freq\\0,2\C,0.036847911,-0.2311357281,0.0171959118\C,0.0439224909,-0.2073504891,1.4140650584\C,1.247187611,-0.1321097971,2.1140918965\C,2.4522242009,-0.0817964712,1.4178025013\C,2.44411445,-0.1037580044,0.0223803182\C,1.2357353119,-0.178832004,-0.6833199311\H,-0.9038412221,-0.2901310007,-0.5206872803\H,-0.8945109446,-0.2480385312,1.9581915315\H,1.2462138156,-0.113541059,3.1987939276\H,3.3952635625,-0.0236262932,1.951179\C,3.7191565144,-0.0538273543,-0.738649471\H,1.2579543487,-0.194666348,-1.768610704\O,3.8725716131,-0.0255203963,-1.9099192844\C,5.7193579958,0.0798102934,0.4847609749\C,6.68411321,0.0604207179,-0.4658676464\H,5.5029196345,-0.8152108207,1.0605034807\H,5.3460992369,1.0270823104,0.8626409216\H,7.1678469528,-0.8570324843,-0.7809168398\C,7.0887980959,1.2550856473,-1.2216855455\O,7.9616310725,1.2670303975,-2.0646071009\O,6.3813548939,2.3552411596,-0.885351192\C,6.7150654766,3.5472902525,-1.604651928\C,5.8061584551,4.6552425901,-1.1116273116\H,6.58479193,3.363398153,-2.6766678912\H,7.7714103952,3.7835524365,-1.4345518028\C,6.0831226837,5.9773361455,-1.8263403373\H,4.7619767017,4.3575520712,-1.2684012917\H,5.9449361853,4.7795769553,-0.0304357782\C,5.1730118406,7.1015964549,-1.3362047164\H,7.1324126625,6.2604268341,-1.6752831851\H,5.9514774623,5.8412939054,-2.907066061\H,5.3811564711,8.0407040232,-1.8558242624\H,4.1202689691,6.8511037328,-1.5024523526\H,5.3089280114,7.273370701,-0.2634796087\\Version=ES64L-G09RevD.01\State=2-A\HF=-769.0220908\S2=0.773784\S2-1=0.\S2A=0.750168\RMSD=2.875e-09\RMSF=2.260e-07\ZeroPoint=0.2813769\Thermal=0.2991857\Dipole=-2.0917739,0.1441251,1.4655462\PG=C01 [X(C14H17O3)]\\@

T rad-nBA TS

1\1\GINC-R3081\Freq\UM062X\6-31+G(d,p)\C15H19O3S1(2)\ROOT\25-Jul-2014\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test G
enChk UM062X/6-31+G(d,p) Freq\\T_BA_TS.4.freq\\0,2\C,0.3726596983,0.174097585,-0.1348535498\C,0.2782311251,0.0638717711,1.2
599299973\C,1.4377226825,-0.1851768565,2.0129980911\C,2.6651362242,-0.3183103577,1.3847206086\C,2.7569305593,-0.210207911
6,-0.0065651402\C,1.604597281,0.0359292681,-0.7609613203\H,-0.5063883218,0.3669330476,-0.7384334385\S,-1.225004103,0.21849
95717,2.166575837\H,1.3679526306,-0.2702566354,3.0932977326\H,3.5571885045,-0.5083936068,1.9724873235\C,4.0562019075,-0.3
542685271,-0.695557532\H,1.6876333375,0.1192207628,-1.8404102157\O,4.2850495454,-0.351606134,-1.8557076982\C,5.9787279832
,-0.3312627083,0.6571520446\C,6.9936068089,-0.2424279013,-0.2337702453\H,5.7423021125,-1.2750978838,1.1381514462\H,5.57169
79323,0.5813748312,1.0853969086\H,7.5189008472,-1.1098512906,-0.6162205072\C,7.3354469598,1.0709913216,-0.8005790574\O,6.
7695008032,2.114150659,-0.5409327037\O,8.366518789,0.9910753283,-1.6647276724\C,8.7568839022,2.2236675775,-2.2796005071\
C,9.9142133918,1.9299326905,-3.2129062645\H,9.0372964288,2.9391318243,-1.4984079007\H,7.897757579,2.6402523033,-2.8170527
131\C,10.4032509612,3.1904872535,-3.9250311313\H,10.7342788405,1.4834547849,-2.637294332\H,9.5979532101,1.1823203714,-3.9
504626339\C,11.5714470304,2.9060910278,-4.8668696555\H,9.5741129737,3.6344252362,-4.4902565439\H,10.7046735814,3.9370356
786,-3.1794098144\H,11.9105932526,3.8152749005,-5.3705531338\H,12.4215263024,2.4881657258,-4.3179755831\H,11.2840270494,2
.1821627602,-5.6361968036\C,-2.4464277625,0.5418392702,0.8736757319\H,-3.3998279086,0.6508762065,1.392376397\H,-2.2267802
518,1.4692594616,0.3412812168\H,-2.5189603852,-0.2938552825,0.1750242215\\Version=ES64L-G09RevD.01\State=2-A\HF=-1206.474
5037\S2=0.772208\S2-1=0.\S2A=0.750144\RMSD=8.840e-09\RMSF=7.828e-07\ZeroPoint=0.3104137\Thermal=0.3315068\Dipole=-1.5234
678,-0.3402255,0.1603096\PG=C01 [X(C15H19O3S1)]\\@

M rad-nBA TS

1\1\GINC-R123\Freq\UM062X\6-31+G(d,p)\C14H26N1O3(2)\ROOT\26-Jul-2014\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test G
enChk UM062X/6-31+G(d,p) Freq\\N_BA_TS.1.freq\\0,2\C,-0.3207181987,-0.508337636,0.2052282561\C,-0.2250377075,-0.2012202719,
1.6934587703\N,1.1452392484,-0.4208872498,2.1642589939\C,1.6085153508,-1.7654110662,1.82435415\C,1.4486698998,-2.00237483
14,0.328467548\O,0.1111767445,-1.8228942197,-0.0831950733\H,0.2886944209,0.2125018035,-0.363721505\H,-1.3590708192,-0.4382
79184,-0.125885996\H,-0.9193278212,-0.8477226032,2.2530976486\H,-0.5035225023,0.8423959156,1.8496294366\H,1.0328928257,-2.
5261472068,2.373728283\H,2.662239705,-1.8726971829,2.0847319613\H,1.722010972,-3.030492238,0.0792386488\H,2.1055673429,-1
.3114488693,-0.224612301\C,1.5605648768,0.1772542096,3.3455757744\C,1.1246532603,1.5975522996,3.5773598148\C,2.905519215
2,-0.2258615372,3.873660423\H,1.4307552801,2.2528937805,2.746806794\H,1.5863840926,1.9795253681,4.4903758686\H,0.0411497
004,1.7033359103,3.6957819087\H,3.7100001417,-0.0400126692,3.1443035958\H,2.938144666,-1.2870838598,4.1459182932\H,3.1362
187033,0.3505345215,4.7722507437\C,0.2139725787,-0.8231585678,5.1690415331\H,0.822674913,-0.2121582087,5.8276827582\H,-0.
647766866,-0.3575159396,4.6988825384\C,0.3283436304,-2.1722027843,5.157881906\C,-0.5946617197,-2.968135157,4.3461792568\H
,1.1122184997,-2.7005444206,5.6896454039\O,-1.5392040932,-2.5335563953,3.7104166384\O,-0.2663550956,-4.2788968176,4.3428371585\C,-1.1072995789,-5.1257021397,3.551007192\C,-0.577006567,-6.541018501,3.6633165458\H,-1.098126536,-4.7693077809,2.5143554937\H,-2.1373319954,-5.049048593,3.9166744656\C,-1.4140014756,-7.5274353338,2.8498708903\H,0.4644646263,-6.5621103983,3
.3191516905\H,-0.5694883615,-6.8381638736,4.7191492169\C,-0.8862768332,-8.9568565275,2.9539050827\H,-2.4549468729,-7.4932117582,3.195159294\H,-1.4263204107,-7.2146087815,1.7982216904\H,-1.4939941094,-9.6519312395,2.36840302\H,0.1436380599,-9.0196509036,2.5878287521\H,-0.890995542,-9.2991803729,3.9938033464\\Version=ES64L-G09RevD.01\State=2-A\HF=-829.1625111\S2=0.
761113\S2-1=0.\S2A=0.750053\RMSD=1.499e-09\RMSF=1.339e-06\ZeroPoint=0.3916991\Thermal=0.4123145\Dipole=0.9679278,0.4234
397,-0.0641663\PG=C01 [X(C14H26N1O3)]\\@

M rad-tBA TS

1\1\GINC-R51\Freq\UM062X\6-31+G(d,p)\C14H26N1O3(2)\ROOT\12-Mar-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test G
enChk UM062X/6-31+G(d,p) Freq\\N_TBA_TS.1.freq\\0,2\C,-0.0886884503,0.1234370104,0.0624209312\C,-0.0347958336,0.1252870609,
1.5833164521\N,1.3551539129,0.0314292932,2.0396529736\C,2.0360220217,-1.1134992007,1.434673835\C,1.8954428263,-1.0640121981,-0.0808340846\O,0.5414862577,-1.0214496885,-0.475492257\H,0.3976972039,1.0309668714,-0.3307171683\H,-1.1271205043,0.1001910205,-0.2751569733\H,-0.6117844439,-0.726949447,1.9749823144\H,-0.4764438693,1.055731443,1.9445773216\H,1.6104392867,-2.0582690528,1.8037714846\H,3.0971937348,-1.0889299573,1.6865352391\H,2.3273997507,-1.963920924,-0.5259532745\H,2.425374993,-0.1802533728,-0.4720716115\C,1.6623357801,0.4040344696,3.3410197175\C,0.9975163513,1.6484366964,3.863010183\C,3.0590006658,0.1236864494,3.812662545\H,1.1917810483,2.5113813461,3.2073430735\H,1.3902791023,1.8872207781,4.8536348699\H,-0.0883833301,1.5485409456,3.9621198192\H,3.8149326128,0.6068999296,3.1737419048\H,3.2746977312,-0.9503706559,3.8369475882\H,3.189143134,0.507681613,4.826803142\C,0.5152270863,-1.1588048912,4.8210437399\H,0.9705875188,-0.6046671372,5.6357344929\H,-0.4136951205,-0.7758355358,4.4074796211\C,0.8855136404,-2.434969705,4.5488989307\C,0.1610275682,-3.1944766196,3.5261228664\H,1.7423547362,-2.9093085967,5.0147297093\O,-0.8305280763,-2.7975879119,2.9357287053\O,0.7541309154,-4.3819503888,3.2837499765\C,0.2457616484,-5.2766590771,2.2543676008\C,1.1721552224,-6.4834375148,2.3650183629\C,0.3855629405,-4.6209517494,0.8813726263\C,-1.1948203692,-5.6869892765,2.5556001646\H,0.9058888045,-7.229352276,1.6108236005\H,2.2113064526,-6.180591043,2.2089288892\H,1.0874666694,-6.9387922352,3.3556933385\H,0.0828751379,-5.3334795456,0.1075467905\H,-0.2334380087,-3.

7260702589,0.7955173756\H,1.4321665564,-4.3512143664,0.702465366\H,-1.4805466562,-6.5034155118,1.8848618619\H,-1.2708086424,-6.0484317387,3.5858400767\H,-1.8845393574,-4.8546520221,2.4183861171\\Version=ES64L-G09RevD.01\State=2-A\HF=-829.1718619\S2=0.762213\S2-1=0.\S2A=0.750058\RMSD=1.220e-09\RMSF=1.973e-06\ZeroPoint=0.3903827\Thermal=0.4106625\Dipole=0.8264333,0.6669427,0.0301061\PG=C01 [X(C14H26N1O3)]\\@

M rad-tBA TS (alt)

1\1\GINC-R157\Freq\UM062X\6-31+G(d,p)\C14H26N1O3(2)\ROOT\19-Apr-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/6-31+G(d,p) Freq\\N_TBA_TS.5.freq\\0,2\C,-0.713357675,0.5116506774,1.3726600127\C,-0.0202516877,0.3187276319,2.7124825169\N,1.403461885,0.028842033,2.5123475448\C,1.5964432589,-1.0781556512,1.5778728172\C,0.8335333248,-0.8223001631,0.2854442122\O,-0.538797452,-0.609223321,0.5288247539\H,-0.3187596568,1.4116820943,0.8743218924\H,-1.7883606447,0.6305175202,1.5231704277\H,-0.5025084196,-0.4908358062,3.2812754112\H,-0.1283696208,1.2355090543,3.2935087079\H,1.2463998407,-2.0242905376,2.0247126819\H,2.6559573958,-1.1793984431,1.3382505594\H,0.910277566,-1.6904998547,-0.3731724906\H,1.2626581515,0.0545696017,-0.2256641873\C,2.2593136141,0.1343456628,3.6050766406\C,1.9994814111,1.2676649216,4.5553829038\C,3.7080069805,-0.1976551365,3.3669253239\H,2.0779251647,2.2381255685,4.0424599914\H,2.7388613876,1.2449956887,5.3583722098\H,1.0143578606,1.2063681286,5.0260477553\H,4.1536785187,0.4785902206,2.6201086488\H,3.869034179,-1.2233845875,3.0234185758\H,4.2626363796,-0.077486503,4.3000543469\C,1.6937171818,-1.7061910474,5.0362681151\H,2.6486306262,-2.1769844991,4.8273475615\H,0.8770054787,-1.8936297726,4.3450393068\C,1.4047644318,-1.2473067247,6.2834384597\C,0.0655409804,-0.7338288523,6.5702452508\H,2.1493068199,-1.1771616594,7.068649445\O,-0.8463729252,-0.6764577523,5.7583731773\O,-0.0365732524,-0.3078575874,7.847747896\C,-1.2665620461,0.2852703552,8.3440072609\C,-0.9232220017,0.6220874656,9.791662728\C,-2.4080651001,-0.7282873087,8.289940147\C,-1.5900733526,1.559675818,7.5650855276\H,-1.7850606318,1.0810948793,10.2842763105\H,-0.6479781891,-0.2849559211,10.3368259322\H,-0.082117233,1.3199541884,9.8307195489\H,-3.2810379942,-0.3150350466,8.8050141954\H,-2.680517101,-0.9630267865,7.2608003963\H,-2.1124980412,-1.6495144844,8.8012730135\H,-2.419142854,2.0809431931,8.0538185672\H,-0.7209550362,2.225554137,7.5631698969\H,-1.8720159794,1.3333468721,6.5362064545\\Version=ES64L-G09RevD.01\State=2-A\HF=-829.1701107\S2=0.765145\S2-1=0.\S2A=0.750078\RMSD=1.355e-09\RMSF=1.953e-06\ZeroPoint=0.3903882\Thermal=0.4107651\Dipole=0.9032267,0.5550514,-0.2502042\PG=C01 [X(C14H26N1O3)]\\@

M rad-tBMA TS

1\1\GINC-R46\Freq\UM062X\6-31+G(d,p)\C15H28N1O3(2)\ROOT\12-Mar-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/6-31+G(d,p) Freq\\N_TBMA_TS.1.freq\\0,2\C,-1.9169532463,2.580643752,-0.7388340203\C,-1.9520394842,1.0891190856,-1.0387400313\N,-2.2075795741,0.3308945855,0.189689932\C,-1.2667454484,0.6963895384,1.2484497583\C,-1.2648965534,2.2052736231,1.4511070084\O,-0.9606355705,2.8891054452,0.2552576522\H,-2.9124838145,2.9193687885,-0.4089619746\H,-1.6306899889,3.1350938729,-1.6353122229\H,-0.9961108182,0.7741338553,-1.4857793239\H,-2.7554200736,0.9045757362,-1.7540646916\H,-0.2463741022,0.3637954972,0.9994153337\H,-1.563713808,0.2228792242,2.1856834485\H,-0.5000545011,2.4842348922,2.1805053679\H,-2.2503330983,2.5281905788,1.824516384\C,-2.6201137644,-0.993628097,0.0804297716\C,-3.6366043692,-1.2960057559,-0.9874659856\C,-2.7675854596,-1.7573172456,1.3676496794\H,-4.5522430483,-0.7001841452,-0.8472549263\H,-3.9153099903,-2.351105475,-0.939045247\H,-3.2683721143,-1.1051793528,-1.9996432203\H,-3.4879437762,-1.2732383873,2.0463931751\H,-1.819428413,-1.8630230346,1.9026026244\H,-3.1369200121,-2.7637006128,1.1573337667\C,-0.8142676758,-2.2557966485,-0.8615840011\H,-1.4163353659,-3.1306834458,-0.6321412708\H,-0.9829570311,-1.7624903021,-1.8139245913\C,0.3437691086,-2.0192239263,-0.1855493477\C,1.1950095792,-0.9206690725,-0.6764035049\C,0.7378065762,-2.7497466976,1.0687686394\O,0.9964063076,-0.2836358631,-1.6986026581\O,2.217303792,-0.6747525574,0.1702236883\C,3.1455662446,0.4208437821,-0.0692562164\C,4.1191327342,0.3016898476,1.0990134619\C,2.4017081946,1.7532119111,-0.0107612838\C,3.8810894997,0.2247070312,-1.3937248969\H,4.8673498711,1.0974875744,1.0449160292\H,3.5844943425,0.3861345487,2.0494142083\H,4.6307686946,-0.6646040727,1.0719633164\H,3.1221082913,2.5738895865,-0.0862237263\H,1.6757396889,1.8462314752,-0.8192363339\H,1.8750020584,1.8502767506,0.944474486\H,4.6965417558,0.9518473866,-1.460172637\H,4.3143034753,-0.7795734184,-1.4343766848\H,3.2130292739,0.3593748807,-2.2440524298\H,0.0332144303,-3.5607001789,1.2724578209\H,1.7429549725,-3.1743576975,0.9848561206\H,0.7565902107,-2.0792852626,1.9372107863\\Version=ES64L-G09RevD.01\State=2-A\HF=-868.4712979\S2=0.766275\S2-1=0.\S2A=0.750084\RMSD=1.794e-09\RMSF=4.304e-06\ZeroPoint=0.4183877\Thermal=0.4401748\Dipole=-0.7190628,-0.1618653,0.7029631\PG=C01 [X(C15H28N1O3)]\\@

9.3 Binding Energy Section

MMMP

1\1\GINC-R113\Freq\RM062X\6-31+G(d,p)\C15H21N1O2S1\ROOT\01-Oct-2015\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\MMMP_7.freq\\0,1\C,-5.0836614858,-0.1366315817,-0.7610487833\C,-3.796929385,-0.5895712241,-0.4959220688\C,-2.8622205941,0.2105758515,0.1713888057\C,-3.2556311499,1.4988291828,0.5688371825\C,-4.5384404274,1.9577552408,0.3068313649\C,-5.4695047299,1.1474332133,-0.3591852647\C,-1.5091815801,-0.4005293451,0.4127256156\O,-1.262165094,-1.4978386925,-0.0522740935\C,-0.4480922508,0.2895302502,1.3061509055\C,0.8469430306,-0.5327018481,1.2574558427\C,-1.0059391747,0.2582956796,2.7418496113\N,-0.2787796771,1.6803012932,0.8474716297\S,-7.0692733841,1.8410570858,-0.6338168711\C,-7.9423735265,0.5087432327,-1.4886280893\C,0.5654915862,2.5293449321,1.6822365167\C,0.4572567057,3.9691982928,1.1939226039\C,0.1455499044,1.7975969199,-0.5463271101\C,0.0357064163,3.2523009669,-0.9798716025\O,0.8360893332,4.08470603,-0.1621079039\H,-5.7754846157,-0.7910435472,-1.278415229\H,-3.4952317597,-1.5849561405,-0.8052499261\H,-2.5417831147,2.1498388131,1.0579855841\H,-4.8247659064,2.9586037567,0.6177507006\H,0.6773409157,-1.533293769,1.6599959155\H,1.6182685601,-0.0421376788,1.858426228\H,1.2112280045,-0.6534328575,0.2350524835\H,-1.3828420523,-0.7438162569,2.96626642\H,-1.822615089,0.9718776505,2.8750051059\H,-0.2180428123,0.4798475831,3.4671102806\H,-8.9469744288,0.8889570805,-1.6789356943\H,-8.0151051017,-0.3841718812,-0.8646278094\H,-7.4689313615,0.2694365751,-2.4428305635\H,1.6267197039,2.2235558273,1.6491266403\H,0.2264276197,2.4863809509,2.7210807707\H,1.1256002532,4.6199341579,1.7628209732\H,-0.5801277547,4.3192792979,1.3214393492\H,-0.5011962869,1.1821378643,-1.1822204567\H,1.1878261462,1.4626894944,-0.6898841243\H,-1.0170035073,3.5724247491,-0.9232774897\H,0.3944780706,3.38082285,-2.0034974502\\Version=ES64L-G09RevD.01\State=1-A\HF=-1187.2781116\RMSD=5.271e-09\RMSF=5.140e-06\ZeroPoint=0.341921\Thermal=0.3607115\Dipole=-0.7219208,0.0142597,0.3219013\PG=C01 [X(C15H21N1O2S1)]\\@

DMPA

1\1\GINC-R3062\Freq\RM062X\6-31+G(d,p)\C16H16O3\ROOT\09-Jan-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\DMPA.freq\\0,1\O,-1.6045310968,-0.2070722201,-2.3047018638\C,-1.8942747915,-0.5207205281,-1.1724709822\C,-3.3258581895,-0.7570814707,-0.7831491895\C,-3.7272564512,-1.3292100041,0.4302689207\C,-5.0818771421,-1.5246730188,0.692301921\C,-6.0418081608,-1.1452290505,-0.2435784885\C,-5.6468148625,-0.5726317698,-1.4534004213\C,-4.2964581458,-0.3846718643,-1.7224818899\C,-0.7641949735,-0.7193491931,-0.1166413206\O,-1.1203016594,-0.1656727423,1.1238514153\O,0.3602743453,-0.090037541,-0.6561675765\C,-0.5288171983,-2.2145070673,0.0774140112\C,-0.5712994773,-2.8171520078,1.3338725313\C,-0.3083808848,-4.1812153878,1.4594285611\C,-0.0027644574,-4.9437066151,0.3340097936\C,0.0456751895,-4.338438566,-0.922058406\C,-0.2148542506,-2.977035997,-1.0506208266\C,-1.3585967664,1.2344142518,1.0907265522\C,1.5407512763,-0.2271487173,0.1193594121\H,-2.9909162789,-1.6228037891,1.1674964208\H,-5.3861150053,-1.9752305845,1.6316004988\H,-7.0959861049,-1.2962052609,-0.0320037069\H,-6.3914200755,-0.2763348626,-2.1852949553\H,-3.9669545496,0.0506991523,-2.660230741\H,-0.8027630371,-2.2149465489,2.206224374\H,-0.3401986805,-4.646905721,2.4395885461\H,0.1990155799,-6.005557963,0.4343313735\H,0.2868245382,-4.9268271286,-1.8016601549\H,-0.1681707478,-2.4932992259,-2.0232395064\H,-1.6050546339,1.5250951456,2.1119014632\H,-2.2033216611,1.4776397364,0.433664085\H,-0.4714465011,1.7762920989,0.7497521587\H,2.2856244398,0.41253501,-0.3542843405\H,1.8957486544,-1.2637956569,0.1216353614\H,1.3778317604,0.0982051076,1.1533469699\\Version=ES64L-G09RevD.01\State=1-A\HF=-844.6720118\RMSD=1.005e-09\RMSF=6.494e-06\ZeroPoint=0.2873608\Thermal=0.3045719\Dipole=-0.2920668,-0.2994092,1.0492983\PG=C01 [X(C16H16O3)]\\@

$AlCl_3$(MMA)

1\1\GINC-R370\Freq\RM062X\6-31+G(d,p)\C5H8Al1Cl3O2\ROOT\12-Aug-2015\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\MMA_mon_AlCl3.1.freq\\0,1\Al,-1.1663362649,-0.0842347404,-0.0999276061\O,0.6773198344,-0.0871398214,-0.1658865161\Cl,-1.6516165295,-2.1356081936,0.1523928117\Cl,-1.7116747898,0.7122923544,-1.9925093683\C,1.8610846606,-0.2198374423,-0.5103926761\C,2.9711068772,0.4558506426,0.1927920562\O,2.2153374635,-0.968941863,-1.5137276939\C,1.1776659024,-1.6642822502,-2.2479880579\C,2.6372419901,1.2420070279,1.2230289489\C,4.3689610646,0.2120925396,-0.3011276724\H,1.7070068987,-2.230972281,-3.0090311892\H,0.5003475937,-0.9359243008,-2.6969529881\H,0.6313855228,-2.3231722661,-1.5712143954\H,1.6012415543,1.3721333928,1.5236456179\H,4.6228997969,-0.8503247169,-0.2522210073\H,5.0812186872,0.7704780458,0.307664157\H,4.4769562954,0.5251407397,-1.3431790664\H,3.4026425399,1.7699584649,1.782621124\Cl,-1.5581290976,1.1641846679,1.5624935216\\Version=ES64L-G09RevD.01\State=1-A\HF=-1968.8136519\RMSD=1.205e-09\RMSF=1.468e-05\ZeroPoint=0.131824\Thermal=0.1464374\Dipole=3.4186571,-0.243331,-0.5620744\PG=C01 [X(C5H8Al1Cl3O2)]\\@

$ZnCl_2(MMA)_2$

1\1\GINC-R164\Freq\RM062X\Gen\C10H16Cl2O4Zn1\ROOT\21-Oct-2015\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/ChkBas Freq\\ZnCl_mon2.2.freq\\0,1\Zn,1.5023729569,0.8797732435,0.1055243408\Cl,2.785704299,0.149879533,1.7450848203\Cl,1.4752194957,2.4555091329,-1.424761687\O,1.1070893265,-0.8933747852,-0.8879394102\C,0.1694485969,-1.678875063,-0.9917719788\O,0.2945648908,-2.9425650592,-0.6298574114\C,1.5917817602,-3.3246212757,-0.1251474414\C,-1.1733686967,-1.3228247298,-1.5164999571\C,-2.3075171654,-2.279544657,-1.2838780383\C,-1.2661197833,-0.162718169,-2.1774742047\H,1.4659980223,-4.3386706457,0.2461451012\H,1.9094009369,-2.6390155202,0.6640772178\H,2.3185244082,-3.2925823816,-0.9382746081\H,-2.4612827559,-2.4411362081,-0.2115035627\H,-2.0997115318,-3.2534768443,-1.7352037626\H,-3.228137802,-1.8789596277,-1.7123075301\H,-0.4035648201,0.4862992376,-2.3181069811\H,-2.2173999631,0.1557462921,-2.5946999099\O,-0.3920880124,1.0150483042,0.9351308076\C,-1.5089702459,0.5227512963,1.042103522\O,-1.7207981227,-0.5987425889,1.7100978367\C,-2.7078324314,1.167214019,0.4446250538\C,-3.9067653938,0.5898509593,0.5683698787\C,-2.4297895782,2.4605209695,-0.2655345165\C,-0.574975015,-1.1657846618,2.3737977992\H,-4.0333970189,-0.3419501006,1.1087275485\H,-4.7876610371,1.0484684467,0.1297759132\H,-2.0859429673,3.2192903169,0.4440385726\H,-3.3302964771,2.824101584,-0.7632491813\H,-1.6240925888,2.3463082379,-0.9979269318\H,-0.9646110518,-1.9930281238,2.9623589969\H,-0.091796465,-0.4160080523,3.0018432111\H,0.1524812304,-1.520735079,1.6411204927\\Version=ES64L-G09RevD.01\State=1-A\HF=-3390.8831913\RMSD=1.930e-09\RMSF=7.241e-06\ZeroPoint=0.2549363\Thermal=0.2779499\Dipole=-3.4383661,-2.5565473,-0.0092306\PG=C01 [X(C10H16Cl2O4Zn1)]\\@

$[AlCl_3(MMMP)]$

1\1\GINC-R751\Freq\RM062X\6-31+G(d,p)\C15H21Al1Cl3N1O2S1\ROOT\21-Feb-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\MMMP_AlCl3.Omor.4.freq\\0,1\C,0.0174387051,-0.007221241,-0.011017875\C,0.0044860794,0.0414074525,1.3774854426\C,1.1905431984,0.0588824241,2.1212125762\C,2.4091499626,0.0306916538,1.4228884883\C,2.4303188318,-0.0106880603,0.0367775798\C,1.2360312214,-0.0328953894,-0.6997269758\C,1.0412788176,0.1253450417,3.6151732985\O,-0.071179913,0.2093563161,4.1000658642\C,2.265935266,0.1476905554,4.5650291706\C,1.7766857248,-0.0194883495,6.0097421133\C,2.9115271007,1.5374916581,4.4127142236\N,3.2048153234,-0.911433414,4.1426655934\S,1.3902453381,-0.0916371034,-2.4551302219\C,-0.3305298883,-0.1169104749,-3.0089023936\C,4.4984422862,-0.9159112763,4.8167280362\C,5.4307659116,-1.8793513788,4.105790749\C,2.6287071651,-2.2529591815,4.1897503766\C,3.5373531672,-3.2128983237,3.4509456244\O,4.8535085797,-3.2146922251,4.0761152611\H,-0.9253859809,-0.0218190235,-0.545051681\H,-0.9390994148,0.0683871756,1.912692939\H,3.3441736782,0.0203578507,1.9674527357\H,3.3822230752,-0.0286488212,-0.4865787389\H,1.1409094425,0.8209056846,6.2934274381\H,2.6323576527,-0.0538943655,6.6906561322\H,1.1840938813,-0.928180049,6.1359742047\H,2.1340793514,2.304464335,4.4669257061\H,3.4344965255,1.6457594658,3.4595046997\H,3.613450857,1.7303895901,5.2290212934\H,-0.2882028793,-0.1572891483,-4.0981278616\H,-0.8587859949,0.7903841042,-2.7097207622\H,-0.8536079656,-1.0025492932,-2.643102312\H,4.4278301264,-1.2009558027,5.8790585273\H,4.9556716278,0.0754454623,4.7550238717\H,6.3926034757,-1.9743780703,4.6108678295\H,5.5838350469,-1.5890168904,3.0615592037\H,1.6563562882,-2.2579804781,3.6846423437\H,2.4823781027,-2.6160373674,5.2203679878\H,3.6866596649,-2.9011231998,2.4124305361\H,3.181541801,-4.2421929114,3.4890179123\Al,5.4085975911,-4.5512998872,5.3124265554\Cl,7.5157444968,-4.3880425315,5.2351365152\Cl,4.565928785,-6.3147786929,4.5083719343\Cl,4.5391203267,-3.892761673,7.1342451841\\Version=ES64L-G09RevD.01\State=1-A\HF=-2810.4445767\RMSD=9.792e-09\RMSF=4.385e-06\ZeroPoint=0.3493365\Thermal=0.3747722\Dipole=-0.9866298,2.2383167,-2.044848\PG=C01 [X(C15H21Al1Cl3N1O2S1)]\\@

thioether-bound [$AlCl_3$(MMMP)]

1\1\GINC-R40\Freq\RM062X\6-31+G(d,p)\C15H21Al1Cl3N1O2S1\ROOT\19-May-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\MMMP_AlCl3.S.1.freq\\0,1\C,-2.9874746543,0.5487984199,0.4953248258\C,-1.783888322,1.2152179349,0.6911616517\C,-0.6438130954,0.8851624201,-0.0510370959\C,-0.7333966675,-0.1181592037,-1.0235115058\C,-1.9410727166,-0.7702923006,-1.2502908218\C,-3.0567663664,-0.4437859429,-0.4807209131\C,0.6085660644,1.670594698,0.2712724017\O,0.5100703719,2.6587560672,0.970512645\C,1.9911686215,1.2820401011,-0.2991338109\C,3.0769840228,2.0050583335,0.5115812637\C,2.0138838491,1.8174081424,-1.7449307544\N,2.1149372644,-0.183394395,-0.2821272326\S,-4.5308574866,-1.4106855083,-0.7869817975\C,-5.8813832035,-0.3866631779,-0.1397280208\C,3.2623979898,-0.7428931542,-0.9906383719\C,3.1129127458,-2.2590066685,-1.0536766528\C,2.0409587087,-0.7678870605,1.0569252442\C,1.9051961897,-2.2789786192,0.9356036769\O,3.0090748836,-2.8228015095,0.2360527752\H,-3.8438871622,0.792728446,1.1136129589\H,-1.7062228462,1.9953510522,1.4407872012\H,0.1426081219,-0.4094161322,-1.5865722895\H,-2.0066945118,-1.5468928044,-2.0062838413\H,2.9794934925,3.0863859856,0.4014069385\H,4.0645397617,1.7038694605,0.1499051005\H,3.0039477747,1.7776579123,1.5775258467\H,1.6683850401,2.8546835007,-1.7543226144\H,1.3744054879,1.2308129377,-2.4096360576\H,3.0331946114,1.8085804513,-2.140239353\H,-6.7992931101,-0.9264245101,-0.376931822\H,-5.8672260028,0.5756067939,-0.6521461451\H,-5.7980637676,-0.2667355271,0.9411540259\H,4.218406834,-0.499852867,-0.4928820205\H,3.2971528276,-0.3545627514,-2.012333396\H,3.9881966743,-2.7115281839,-1.5256422996\H,2.2163232264,-2.5108355202,-1.6434932156\H,1.1688992003,-0.3681890674,1.5880684045\H,2.9405389206,-0.5395002967,1.6545104331\H,0.9679586974,-2.5250020526,0.4118336502\H,1.8961378391,-2.7486985098,1.9212848129\Al,-4.3490459543,-3.1155466024,0.9106846295\Cl,-2.5728387544,-4.0877696115,0.3207239669\Cl,-6.1866537381,-4.1102264147,0.5933913965\Cl,-4.2536408616,-1.9739742656,2.6943061829\\Version=ES64L-G09RevD.01\State=1-A\HF=-2810.4259846\RMSD=7.551e-09\RMSF=2.422e-06\ZeroPoint=0.3483246\Thermal=0.3740366\Dipole=0.2169051,1.9354855,-1.6880494\PG=C01 [X(C15H21Al1Cl3N1O2S1)]\\@

(amine,ketone)-bound [$AlCl_3$(MMMP)]

1\1\GINC-R2114\Freq\RM062X\6-31+G(d,p)\C15H21Al1Cl3N1O2S1\ROOT\17-Feb-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\MMMP_AlCl3.OacN.1.freq\\0,1\C,-2.2670662477,3.4010994316,1.3451239461\C,-1.4903423484,2.2868194674,1.0687758414\C,-0.2559215322,2.405359069,0.4107556863\C,0.1665907883,3.6847291157,0.0083756132\C,-0.6112986914,4.797730943,0.26819164\C,-1.8360195334,4.6744367743,0.9482417714\C,0.4715978908,1.1540510756,0.1457672961\O,-0.1127779375,0.0856065313,0.3421362292\C,1.9120706675,1.0537250872,-0.3795111479\C,2.8358772152,2.0925860705,0.2956716189\C,1.8813638519,1.2890985293,-1.9043143339\N,2.3251605673,-0.3852483068,-0.091051458\S,-2.7283541504,6.1593555724,1.2324844475\C,-4.226341916,5.5803608814,2.0635094463\C,3.598433467,-0.6951603756,-0.8270676172\C,4.3553433366,-1.914916869,-0.3009683504\C,2.546726983,-0.5629984034,1.3884568649\C,3.2721945582,-1.859358605,1.7108592368\O,4.543938236,-1.8491326653,1.096991071\H,-3.2093212458,3.2673847901,1.8622860464\H,-1.8332707206,1.2996046357,1.3596898348\H,1.0917603709,3.8259590579,-0.5344920982\H,-0.2771640482,5.7766429417,-0.0617803204\H,2.8851385256,2.9998539762,-0.3065102941\H,3.8567142819,1.7142621101,0.3689879204\H,2.5047835698,2.3676981158,1.2995076361\H,1.3116414369,2.194099986,-2.1281272628\H,1.4060123115,0.4633468029,-2.4395279152\H,2.8983812847,1.4272737871,-2.2789844354\H,-4.8211293677,6.4753838266,2.2500402117\H,-3.9940037766,5.105887534,3.0185867933\H,-4.7971573167,4.9036426164,1.4251435316\H,4.2682544682,0.16744754,-0.7456555062\H,3.3566472623,-0.8611440996,-1.8774607292\H,5.3448463398,-1.9180486094,-0.764523462\H,3.8356801785,-2.8395073737,-0.5653549398\H,1.5803327322,-0.5327398256,1.8952084725\H,3.176791707,0.2490542882,1.7614873992\H,2.6952230561,-2.7368553139,1.3910102712\H,3.4242325069,-1.9155719373,2.7910501391\Al,0.5471716515,-1.589574328,-0.6004655388\Cl,-0.8965891296,-0.9746349118,-2.1168135179\Cl,1.6501349601,-3.0175507335,-1.8335245715\Cl,-0.0613262437,-2.7420281995,1.1155345334\\Version=ES64L-G09RevD.01\State=1-A\HF=-2810.4361682\RMSD=2.522e-09\RMSF=3.864e-06\ZeroPoint=0.3515119\Thermal=0.3760691\Dipole=0.6267442,4.7118356,1.4833521\PG=C01 [X(C15H21Al1Cl3N1O2S1)]\\@

ketone-bound [$AlCl_3$(MMMP)]

1\1\GINC-R1269\Freq\RM062X\6-31+G(d,p)\C15H21Al1Cl3N1O2S1\ROOT\23-Feb-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\MMMP_AlCl3.Oac.5.freq\\0,1\C,-3.0730086666,0.7320913521,0.4038228097\C,-1.8879435015,1.4120304425,0.6222402415\C,-0.6873259317,1.0004853367,0.0123021734\C,-0.7141491891,-0.1329558435,-0.8308211505\C,-1.8994878821,-0.7984191608,-1.0666169102\C,-3.0964575728,-0.3779217645,-0.4536817924\C,0.5048939438,1.7994078881,0.2514588263\O,0.3944437946,2.9417866353,0.7598476996\C,1.9330730417,1.4044936552,-0.1352942999\C,2.9368431517,2.2367871993,0.6830746667\C,2.0337434131,1.8326920293,-1.6194981873\N,2.1000602944,-0.0453614228,0.0142263385\S,-4.5331801209,-1.3070704152,-0.8253791416\C,-5.8331038708,-0.4319668464,0.0775760089\C,3.27922199,-0.6262705761,-0.624312097\C,3.1869808269,-2.1457378187,-0.5393315537\C,2.026114822,-0.5002000792,1.4031873783\C,1.9489501369,-2.0196636602,1.4268659945\O,3.0816847089,-2.5859191507,0.7981677918\H,-3.9719698638,1.0776152503,0.8988263806\H,-1.8914720421,2.2644335501,1.2946285114\H,0.1999864493,-0.481515746,-1.2917413148\H,-1.912726696,-1.6555122283,-1.7330730281\H,2.8654421626,3.2962873713,0.4302063459\H,3.9486622465,1.8911873033,0.4532989773\H,2.7678947604,2.1396571683,1.7581306663\H,1.6510296374,2.850548579,-1.7406039259\H,1.4655315034,1.1661088396,-2.2730499305\H,3.0816548631,1.8373195307,-1.9298816244\H,-6.7566636858,-0.9652311476,-0.1509540485\H,-5.9252498063,0.5998422319,-0.2658319923\H,-5.6624499381,-0.4665889842,1.1549472032\H,4.2175139633,-0.2975548375,-0.1433165174\H,3.3128326944,-0.3404863029,-1.6788521028\H,4.0864887588,-2.6072828913,-0.9526279064\H,2.3111156845,-2.4888997298,-1.113

901985\H,1.1304714453,-0.0828610643,1.8793239575\H,2.9067867145,-0.1809922309,1.9860262818\H,1.0304105897,-2.3489974867,0.9150975445\H,1.9403288844,-2.3914695653,2.4535806101\Al,-0.410685352,4.5873215103,0.5513661084\Cl,-1.6548320704,4.8166973565,2.2558911107\Cl,1.2376490432,5.9117505232,0.4297789484\Cl,-1.4591913348,4.3384832,-1.2857650666\\Version=ES64L-G09RevD.01\State=1-A\HF=-2810.4445081\RMSD=4.651e-09\RMSF=3.100e-06\ZeroPoint=0.348926\Thermal=0.3743237\Dipole=-0.2934312,-3.3124779,-0.5002616\PG=C01 [X(C15H21Al1Cl3N1O2S1)]\\@

(ether,amine,ketone)-bound [$AlCl_3$(MMMP)]

1\1\GINC-R1979\Freq\RM062X\6-31+G(d,p)\C15H21Al1Cl3N1O2S1\ROOT\17-Feb-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\MMMP_AlCl3.Tridendate.3.freq\\0,1\C,-3.8941774279,-0.9835979055,0.9851396834\C,-2.5834399909,-0.9498970659,0.5277716\C,-1.9839811858,0.2463179714,0.1144725288\C,-2.748514856,1.421520314,0.1723769762\C,-4.0631394447,1.3934686534,0.6106986241\C,-4.6536928208,0.1907760014,1.0273053671\C,-0.5720082305,0.1102424013,-0.3616777435\O,-0.1856784233,-0.9742889729,-0.7541740697\C,0.4201588427,1.3043642583,-0.4032777186\C,0.3987746648,2.1538542915,0.8777830198\C,-0.0108006759,2.1780634269,-1.6029565652\N,1.8340057893,0.7227565883,-0.6038818029\S,-6.3254376358,0.2803296912,1.5783291596\C,-6.6887683852,-1.4313413374,2.0332846312\C,2.859703866,1.8081366725,-0.4126215934\C,4.2573784326,1.3089016378,-0.854404855\C,2.0287197873,0.2431212974,-2.0240330392\C,3.4346023835,-0.3679793641,-2.2092502625\O,4.2349644555,-0.0807878026,-1.0850475517\H,-4.3096349879,-1.9296651034,1.3109641387\H,-1.99068244,-1.8581659301,0.5028186567\H,-2.3441924817,2.3790101097,-0.131501315\H,-4.6402841086,2.3130694479,0.6360034767\H,-0.6250389552,2.2637624366,1.2333147015\H,0.7987938052,3.1519774246,0.6778095607\H,0.9627331788,1.696126443,1.6918295743\H,-0.8800593148,2.7721682292,-1.3249897986\H,-0.2766978472,1.5852638941,-2.4810327349\H,0.7733865738,2.88652111,-1.8807069512\H,-7.7200313068,-1.4283310819,2.3887105409\H,-6.0380473581,-1.7744433401,2.839798419\H,-6.6141069375,-2.097008664,1.1713485198\H,2.8811906561,2.0915325034,0.6367240534\H,2.5661964152,2.67896693,-1.0075340678\H,4.9845551643,1.4867029647,-0.0631603369\H,4.5824512607,1.8284767365,-1.7676897082\H,1.9176703272,1.114354645,-2.67576654\H,1.2579910171,-0.4854671426,-2.2604745661\H,3.89977374,0.0423779264,-3.1171348524\H,3.3892417276,-1.4520177456,-2.2861611036\Al,2.2320147513,-0.7971169331,0.8030517638\Cl,3.8406728898,-0.0368324015,2.0098351192\Cl,0.6038506412,-0.9080279277,2.2185994707\Cl,2.5389344449,-2.6788652884,-0.1264624092\\Version=ES64L-G09RevD.01\State=1-A\HF=-2810.423244\RMSD=5.049e-09\RMSF=9.396e-06\ZeroPoint=0.3514529\Thermal=0.376137\Dipole=-1.7993977,2.5975352,-2.1110694\PG=C01 [X(C15H21Al1Cl3N1O2S1)]\\@

amine-bound [$AlCl_3$(MMMP)]

1\1\GINC-R522\Freq\RM062X\6-31+G(d,p)\C15H21Al1Cl3N1O2S1\ROOT\22-Feb-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\MMMP_AlCl3.N.8.freq\\0,1\C,-1.013177374,4.7504903064,1.8600327422\C,-0.1392030171,3.6834081932,1.7712107664\C,0.5036894092,3.3793647335,0.5563279698\C,0.2712443005,4.2056117972,-0.5494516473\C,-0.584542533,5.296573468,-0.4555886092\C,-1.248052027,5.5746189182,0.7462160404\C,1.418911824,2.2172038417,0.5972432901\O,1.9714653992,1.9833336675,1.6685986296\C,1.731071686,1.274932639,-0.5769319766\C,2.8870666135,1.95947974,-1.3355292297\C,0.5149406936,1.151066743,-1.5055177805\N,2.1945439651,-0.0311301686,0.0533102665\S,-2.3714597765,6.907757699,0.9754110787\C,-2.3718026956,7.7195352502,-0.639880826\C,1.0727386881,-0.9757638442,0.4064592253\C,3.1855354537,-0.805528418,-0.7671276334\H,-1.5147052764,4.9593953413,2.8001677771\H,0.0546562074,3.0574201382,2.6374562405\H,0.7815482715,4.0436874187,-1.4919014821\H,-0.7219702176,5.9266550201,-1.32595969\H,2.6079951787,2.9871491478,-1.577048844\H,3.0828471711,1.4420547867,-2.2783981795\H,3.7958637588,1.9937150749,-0.7298408193\H,0.2891694098,2.1217782919,-1.9429047604\H,-0.3825987841,0.8161167252,-0.9809830594\H,0.7241802159,0.4706349408,-2.3287932256\H,-3.0572753418,8.5624621244,-0.5432302746\H,-2.7418231285,7.0534429708,-1.42169588\H,-1.3807409272,8.0999173638,-0.8946801672\C,0.5642733548,-1.8608891971,-0.7360803193\H,0.2578247803,-0.4055812924,0.86353393\H,3.9840040874,-0.143915964,-1.0989492252\C,2.5663009989,-1.5926635916,-1.9106769364\O,1.6197088651,-2.5146779488,-1.4090416697\H,1.4744604223,-1.6419822243,1.1763563729\H,3.6333068046,-1.5311763329,-0.0884445484\H,-0.0541761267,-1.3165715548,-1.4584688141\H,-0.0537049372,-2.64585839,-0.2935894618\H,3.3505123004,-2.1827491548,-2.3904947856\H,2.1093446563,-0.9539393333,-2.6815285498\Al,3.0397106503,0.3327846482,2.0239159465\Cl,1.6083919085,0.1270902869,3.6611058992\Cl,4.8123236394,1.5489349619,1.75959272\Cl,3.9593314482,-1.6477588239,2.2599195\\Version=ES64L-G09RevD.01\State=1-A\HF=-2810.4272178\RMSD=8.811e-09\RMSF=1.132e-05\ZeroPoint=0.3513556\Thermal=0.3758352\Dipole=-3.0109006,2.8108597,-4.245229\PG=C01 [X(C15H21Al1Cl3N1O2S1)]\\@

[$AlCl_3$(DMPA)]

1\1\GINC-R397\Freq\RM062X\6-31+G(d,p)\C16H16Al1Cl3O3\ROOT\16-Jan-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\DMPA_AlCl3.freq\\0,1\O,0.1609825794,0.0961616444,0.0015697905\C,0.1289583367,0.0109737925,1.2388367966\C,1.3961243319,-0.0181944973,1.9710461176\C,1.4564028932,-0.1449605798,3.3690184114\C,2.6933243014,-0.1754172346,4.0008963811\C,3.8657949002,-0.078919081,3.2506373369\C,3.8104793188,0.0458370982,1.8607272344\C,2.5812611984,0.0754062077,1.2188261254\C,-1.2526894794,-0.0480788494,1.9449712584\O,-1.3153332908,-1.1443121561,2.804800943\O,-2.1362054057,-

0.1596248933,0.8784778698\C,-1.4672482819,1.2319706645,2.7426525118\C,-1.7221816243,1.2075530037,4.112874909\C,-1.9371885593,2.404291162,4.7950216849\C,-1.8957056754,3.6186943736,4.1121246202\C,-1.6498914342,3.6382503903,2.7395280142\C,-1.4380814334,2.4462685671,2.0521637819\C,-1.1816087769,-2.4104747489,2.1550668627\C,-3.5290063817,-0.089162755,1.1767429523\H,0.5471005891,-0.2269712552,3.9505908634\H,2.743810985,-0.2734659882,5.0798030733\H,4.8287047756,-0.1019122658,3.7515760737\H,4.7246612279,0.1192394668,1.2819251084\H,2.5163524674,0.1696723625,0.1394053821\H,-1.763144211,0.2571907387,4.6345730135\H,-2.1421926852,2.3858461863,5.8606495257\H,-2.0626098994,4.5482075121,4.6469913135\H,-1.6305994999,4.5794139211,2.2001397459\H,-1.285686066,2.4579697742,0.9747199936\H,-1.2923664621,-3.1600656964,2.937168299\H,-0.1901705409,-2.5122145779,1.6939600921\H,-1.9456334178,-2.5404206887,1.3845069841\H,-4.034875179,-0.4388727152,0.2769923405\H,-3.8184104434,0.9428185077,1.3934854788\H,-3.7669717132,-0.7395083075,2.024073409\Al,-1.051312328,-0.0048012022,-1.4571332124\Cl,0.4539108734,0.1785172549,-2.9627158837\Cl,-1.9319810527,-1.9469860604,-1.5528097608\Cl,-2.3330930463,1.7018578362,-1.5206807627\\Version=ES64L-G09RevD.01\State=1-A\HF=-2467.8428649\RMSD=9.783e-10\RMSF=5.697e-06\ZeroPoint=0.2941887\Thermal=0.3181621\Dipole=1.205515,0.1203498,4.5080181\PG=C01 [X(C16H16Al1Cl3O3)]\\@

(ether,ketone)-bound [$AlCl_3$(DMPA)]

1\1\GINC-R427\Freq\RM062X\6-31+G(d,p)\C16H16Al1Cl3O3\ROOT\15-Feb-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\DMPA_AlCl3.Bidentate.freq\\0,1\O,0.0181347818,-0.2166859693,-0.0011622286\C,-0.0235861178,-0.1106559181,1.21903846\C,1.2078480099,-0.0220626063,2.0171097115\C,1.2003075401,0.0421998899,3.4181586106\C,2.4058807098,0.1127625959,4.1074117024\C,3.6126151155,0.1219771824,3.4081723126\C,3.622078244,0.0565152584,2.0135634383\C,2.4241179796,-0.0176161495,1.316596195\C,-1.4227533537,-0.0647975299,1.8611298008\O,-1.5829745942,-1.0411132247,2.821559124\O,-2.3168500464,-0.3008119707,0.7506672045\C,-1.6897952225,1.3094207885,2.4483204449\C,-2.0447788293,1.4710694922,3.7864848751\C,-2.2942024488,2.7501595306,4.2809031326\C,-2.186592421,3.8587900661,3.4428824422\C,-1.83435212,3.6908648184,2.1040183446\C,-1.5849761395,2.4165842592,1.6021143019\C,-1.3508799829,-2.3807132814,2.3661293168\C,-3.724810176,-0.2505518914,1.1262641271\H,0.2647489121,0.0302228817,3.9640765263\H,2.403875004,0.1618786866,5.1909450236\H,4.5503127591,0.1796506895,3.9520377108\H,4.5625192206,0.0627069055,1.4733000527\H,2.4071586342,-0.0718862215,0.2331125482\H,-2.1310026852,0.601541087,4.4300372158\H,-2.5757450419,2.8786840455,5.3209942669\H,-2.3810447582,4.8531578179,3.8317333473\H,-1.7556976756,4.5498045833,1.4461039668\H,-1.3247946938,2.2875369222,0.5520450262\H,-1.5065787285,-3.018365059,3.2343603364\H,-0.3247473352,-2.4997545256,1.9993664216\H,-2.0487313264,-2.6471007026,1.567772796\H,-4.1436818086,0.6879622243,0.7648232267\H,-3.7873487306,-0.3238992396,2.2111467337\H,-4.2132354818,-1.0941126543,0.6470760505\Al,-1.6652206104,-0.5007999995,-1.1431235615\Cl,-0.8826284656,-2.4904045798,-1.4340381166\Cl,-3.6905632631,-0.7110608663,-1.9122630758\Cl,-1.0780931901,1.354340978,-2.0806490924\\Version=ES64L-G09RevD.01\State=1-A\HF=-2467.8377632\RMSD=8.429e-09\RMSF=3.422e-06\ZeroPoint=0.2950305\Thermal=0.3185913\Dipole=1.3419769,0.8542676,4.8630569\PG=C01 [X(C16H16Al1Cl3O3)]\\@

ether-bound [$AlCl_3$(DMPA)]

1\1\GINC-R1453\Freq\RM062X\6-31+G(d,p)\C16H16Al1Cl3O3\ROOT\15-Feb-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/6-31+G(d,p) Freq\\DMPA_AlCl3.OCH3.2.freq\\0,1\O,-0.6803137356,-1.4045889075,1.8278848667\C,-0.684813921,-0.8996181192,0.7314036669\C,-1.8256163554,-0.0255829747,0.2921099703\C,-2.1239944597,0.3223275086,-1.0318897633\C,-3.227473211,1.1239504564,-1.3125130838\C,-4.0386658959,1.5907828045,-0.2806416635\C,-3.7492124223,1.2465714166,1.0398875765\C,-2.6545117675,0.4390426716,1.3231331094\C,0.6182417049,-1.0756775277,-0.1298116594\O,0.2735464222,-1.377270272,-1.5337465249\O,1.2749355357,-2.1515623447,0.4016595088\C,1.3610501186,0.2461960465,-0.0494788316\C,1.0406333897,1.3332967184,-0.8646976559\C,1.7039733426,2.5454557652,-0.6992242513\C,2.6711998214,2.6847938472,0.2930342221\C,2.9663692053,1.6102028316,1.1307866804\C,2.3065698797,0.3960226369,0.9679657242\C,-0.6370937694,-2.5147364275,-1.646340183\C,2.4965156274,-2.5450440574,-0.2261766532\H,-1.5167396729,-0.0194152803,-1.8604248125\H,-3.4467138991,1.3814136753,-2.3436786817\H,-4.8944792263,2.2198932906,-0.5043767887\H,-4.3766739271,1.6074340558,1.848264477\H,-2.4192613168,0.1575054951,2.3438849568\H,0.2918400433,1.2459337648,-1.6457427073\H,1.4650272325,3.3773753315,-1.3530572716\H,3.1896677715,3.6299168305,0.4178928535\H,3.7092407814,1.7167187172,1.9144346646\H,2.5152803032,-0.4394058996,1.6291930814\H,-1.0511555075,-2.4882884241,-2.6537479328\H,-1.4360384265,-2.3950073544,-0.9155436103\H,-0.0842982757,-3.4377403915,-1.4762806285\H,2.9502669651,-3.2681383294,0.450540576\H,3.169241252,-1.6968056618,-0.3761393098\H,2.3004514716,-3.0303408621,-1.1893533191\Al,1.290916118,-1.0742320234,-3.1770423266\Cl,-0.1454257044,0.0987006642,-4.2173569925\Cl,1.4805633517,-3.0476825169,-3.944458116\Cl,3.1787111562,-0.1957471546,-2.8474531674\\Version=ES64L-G09RevD.01\State=1-A\HF=-2467.8241995\RMSD=1.140e-09\RMSF=7.279e-06\ZeroPoint=0.295147\Thermal=0.3183656\Dipole=-0.9261249,0.7180589,1.4198825\PG=C01 [X(C16H16Al1Cl3O3)]\\@

[$ZnCl_2$(DMPA)]

1\1\GINC-R3474\Freq\RM062X\Gen\C15H21Cl2N1O2S1Zn1\ROOT\21-Feb-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/ChkBas Freq\\MMMP_ZnCl2.OacN.5.freq\\0,1\C,-3.9074382578,-0.6744195187,-0.9847696217\C,-2.5500399305,-0.8128

014604,-0.7289081077\C,-1.8966361526,0.0267426455,0.1832977329\C,-2.6504882048,0.9925740189,0.8689229219\C,-4.009448007,1.1150483416,0.6385648652\C,-4.6547725443,0.2934064145,-0.3019876624\C,-0.4539169041,-0.2277563839,0.386522254\O,-0.0508239937,-1.3795608077,0.2304658012\C,0.5781268282,0.8434827802,0.8062662356\C,0.7171870832,0.6587515777,2.3322688919\C,0.1416719623,2.2872995218,0.5043639678\N,1.8663012616,0.4822723713,0.1074825334\S,-6.3783110288,0.5615953549,-0.5271091065\C,-6.82518595,-0.6930829146,-1.7498465751\C,3.0503474665,1.0714335613,0.7800902936\C,1.8289013273,0.8933553422,-1.3237143061\H,-4.3726446965,-1.3285814204,-1.712194905\H,-1.9731313238,-1.5743550384,-1.2445251813\H,-2.1958529942,1.6272234622,1.6195770143\H,-4.5853017615,1.8494737035,1.1935753142\H,-0.2756861981,0.6896831258,2.7911103668\H,1.3038594751,1.4755097883,2.7602586499\H,1.1867680179,-0.2950893042,2.5879271934\H,-0.5010168274,2.6691168364,1.2974501201\H,-0.391788263,2.3864404562,-0.4435074291\H,1.019401887,2.9378972786,0.4767954535\H,-7.8963498429,-0.571437368,-1.9156570414\H,-6.6386238881,-1.6999685258,-1.3719044367\H,-6.3019741254,-0.5333165174,-2.6944264573\C,4.3110680036,0.7873364595,-0.0206034719\H,3.1531632669,0.6155003854,1.7662205895\H,1.0431580336,0.3171064271,-1.8278483733\C,3.1662733672,0.6504028651,-2.0162725293\Zn,1.9959130202,-1.7061135407,0.1469506011\Cl,3.0650998529,-2.1605842954,2.0342287371\Cl,2.136359391,-2.6894971288,-1.8355753895\O,4.2084329934,1.311401805,-1.3265403197\H,2.9370860785,2.1600282127,0.881641989\H,1.6037840162,1.9622650134,-1.4063998025\H,4.5030863039,-0.2975926805,-0.0548053795\H,5.1638063996,1.2705146367,0.4602416097\H,3.1245716469,1.0726670333,-3.0225057881\H,3.3828632116,-0.4210625139,-2.0974212518\\Version=ES64L-G09RevD.01\State=1-A\HF=-3886.8586729\RMSD=2.372e-09\RMSF=1.071e-05\ZeroPoint=0.3479769\Thermal=0.3716111\Dipole=-3.4502464,3.0857694,0.0106505\PG=C01 [X(C15H21Cl2N1O2S1Zn1)]\\@

(ether,amine,ketone)-bound [$ZnCl_2$(MMMP)]

1\1\GINC-R389\Freq\RM062X\Gen\C15H21Cl2N1O2S1Zn1\ROOT\22-Oct-2015\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/ChkBas Freq\\MMMP_7_ZnCl2_3.freq\\0,1\C,-5.295396408,-0.0248179135,-1.0846030148\C,-3.9262587636,-0.0577873201,-0.8523848967\C,-3.4064146029,0.1930271368,0.4237145618\C,-4.2952183092,0.4418706277,1.4800334752\C,-5.6621162402,0.4457300243,1.2590096211\C,-6.1799613202,0.2260026711,-0.0287809199\C,-1.9313626048,0.1208611317,0.5467220275\O,-1.3295038235,-0.6544762517,-0.185411104\C,-1.0948401913,0.9568939927,1.5470198225\C,-0.8168205246,-0.0189884366,2.7065177506\C,-1.7929232383,2.2199206532,2.0710516705\N,0.166884009,1.2834197462,0.8212551176\S,-7.9326557964,0.2818675945,-0.1902109393\C,-8.1883517439,-0.10753471,-1.9371712014\C,1.3230963456,1.5951601114,1.6797690308\C,2.5890411687,1.6310534268,0.7832646568\C,-0.0067468357,2.3740338697,-0.1625233885\C,1.3237729931,2.5391035182,-0.9437180905\O,2.2145388881,1.4945136306,-0.5788708176\H,-5.6604796621,-0.2033058563,-2.0888439077\H,-3.2358219759,-0.2705441397,-1.6639800412\H,-3.9339358428,0.5900787693,2.4909858167\H,-6.3418615327,0.6134432624,2.0891000265\H,-1.759258445,-0.4630490634,3.0415861408\H,-0.3808464837,0.5083015208,3.5593554633\H,-0.1481890545,-0.8246794945,2.3877972086\H,-2.4906503194,1.9817320537,2.8739307997\H,-2.3410854567,2.7569913408,1.2928455426\H,-1.0423756729,2.8933331913,2.4965480915\H,-9.2692961392,-0.1034242959,-2.0830277615\H,-7.8024989282,-1.098574204,-2.1831664363\H,-7.742364682,0.6497500587,-2.5845627624\H,1.443216089,0.8029585709,2.4172785395\H,1.1750137394,2.5539689224,2.1997418502\H,3.2368732816,0.7821950778,1.0008861681\H,3.144194544,2.5679839313,0.9152311407\H,-0.2786412291,3.3153487242,0.3329624263\H,-0.8119187467,2.0889705893,-0.850020137\H,1.7967202321,3.5036698489,-0.7201571102\H,1.1614595173,2.4438041305,-2.0164552153\Zn,0.7740539491,-0.3766192325,-0.5516858918\Cl,1.9591105035,-1.7221320391,0.7651890197\Cl,0.3588493129,-0.07896517,-2.7309323324\\Version=ES64L-G09RevD.01\State=1-A\HF=-3886.8533919\RMSD=6.448e-10\RMSF=8.548e-06\ZeroPoint=0.3475811\Thermal=0.3714662\Dipole=-2.7675336,2.9126665,1.9681651\PG=C01 [X(C15H21Cl2N1O2S1Zn1)]\\@

(ether,amine)-bound [$ZnCl_2$(MMMP)]

1\1\GINC-R3474\Freq\RM062X\Gen\C15H21Cl2N1O2S1Zn1\ROOT\21-Feb-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/ChkBas Freq\\MMMP_ZnCl2.OacN.5.freq\\0,1\C,-3.9074382578,-0.6744195187,-0.9847696217\C,-2.5500399305,-0.8128014604,-0.7289081077\C,-1.8966361526,0.0267426455,0.1832977329\C,-2.6504882048,0.9925740189,0.8689229219\C,-4.009448007,1.1150483416,0.6385648652\C,-4.6547725443,0.2934064145,-0.3019876624\C,-0.4539169041,-0.2277563839,0.386522254\O,-0.0508239937,-1.3795608077,0.2304658012\C,0.5781268282,0.8434827802,0.8062662356\C,0.7171870832,0.6587515777,2.3322688919\C,0.1416719623,2.2872995218,0.5043639678\N,1.8663012616,0.4822723713,0.1074825334\S,-6.3783110288,0.5615953549,-0.5271091065\C,-6.82518595,-0.6930829146,-1.7498465751\C,3.0503474665,1.0714335613,0.7800902936\C,1.8289013273,0.8933553422,-1.3237143061\H,-4.3726446965,-1.3285814204,-1.712194905\H,-1.9731313238,-1.5743550384,-1.2445251813\H,-2.1958529942,1.6272234622,1.6195770143\H,-4.5853017615,1.8494737035,1.1935753142\H,-0.2756861981,0.6896831258,2.7911103668\H,1.3038594751,1.4755097883,2.7602586499\H,1.1867680179,-0.2950893042,2.5879271934\H,-0.5010168274,2.6691168364,1.2974501201\H,-0.391788263,2.3864404562,-0.4435074291\H,1.019401887,2.9378972786,0.4767954535\H,-7.8963498429,-0.571437368,-1.9156570414\H,-6.6386238881,-1.6999685258,-1.3719044367\H,-6.3019741254,-0.5333165174,-2.6944264573\C,4.3110680036,0.7873364595,-0.0206034719\H,3.1531632669,0.6155003854,1.7662205895\H,1.0431580336,0.3171064271,-1.8278483733\C,3.1662733672,0.6504028651,-2.0162725293\Zn,1.9959130202,-1.7061135407,0.1469506011\Cl,3.0650998529,-2.1605842954,2.0342287371\Cl,2.136359391,-2.6894971288,-1.8355753895\O,4.2084329934,1.311401805,-1.3265403197\H,2.9370860785,2.1600282127,0.881641989\H,1.6037840162,1.9622650134,-1.4063998025\H,4.5030863039,-0.2975926805,-0.0548053795\H,5.1638063996,1.2705146367,0.4602416097\H,3.1245716469,1.0726670333,-3.0225057881\H,3.3828632116,-0.4210625139,-2.0974212518\\Version=ES64L-G09RevD.01\State=1-A\HF=-3886.8586729\RMSD=2.372e-09\RM

SF=1.071e-05\ZeroPoint=0.3479769\Thermal=0.3716111\Dipole=-3.4502464,3.0857694,0.0106505\PG=C01 [X(C15H21Cl2N1O2S1Zn1)]\\@

ketone-bound [$ZnCl_2$(MMMP)(MMA)]

1\1\GINC-R1014\FOpt\RM062X\Gen\C20H29Cl2N1O4S1Zn1\ROOT\20-Feb-2016\0\\#M062X/gen 6D 10F INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=939524096\\MMMP_ZnCl2.Oac.MMA.2c.freq\\0,1\C,1.9715685266,3.0833417319,0.3757048046\C,1.1883268465,1.9409558108,0.300422403\C,1.7600167347,0.6596989715,0.338162271\C,3.1577108276,0.5547608112,0.4585233148\C,3.9429305887,1.6927168987,0.5320763492\C,3.3636213212,2.9716056624,0.4917893391\C,0.8193979809,-0.4869158262,0.2939225877\O,-0.371742928,-0.2282550069,0.0997008674\C,1.240306512,-1.9423389208,0.5643794165\C,0.067549653,-2.8977092481,0.2939530938\C,1.5795339247,-1.9885156565,2.0684837491\N,2.423987651,-2.2297400343,-0.2636861952\S,4.4656238071,4.3391710559,0.5957862717\C,3.3518755518,5.7622889149,0.5378498234\C,3.1499646367,-3.4542510246,0.0628554337\C,4.4360294239,-3.4984295311,-0.7540298395\C,2.1473070167,-2.1929658593,-1.7000069162\C,3.4613525946,-2.2583879662,-2.4646889987\O,4.1722661189,-3.4367880682,-2.1402598041\H,1.4896741037,4.0533702794,0.3508371461\H,0.1090736917,2.0279623379,0.2253973435\H,3.6199649566,-0.4238255562,0.4678496985\H,5.0210525323,1.5960647618,0.6212379455\H,-0.6898465644,-2.8200458875,1.0798255539\H,0.4371029298,-3.9269262938,0.3149703289\H,-0.4113627428,-2.7224448773,-0.6728273907\H,0.7655208945,-1.530778955,2.6398732163\H,2.5125771074,-1.4640261628,2.2894947227\H,1.6613228753,-3.0273216341,2.3991588081\H,3.9947680031,6.6407810062,0.6070520667\H,2.6623972017,5.7618228815,1.3841626299\H,2.8025717384,5.8005062016,-0.4047096095\H,2.559132604,-4.3612129248,-0.1558184819\H,3.4112067316,-3.4599696082,1.1244394323\H,4.9704218142,-4.4344941861,-0.5770321048\H,5.0832051481,-2.6553028397,-0.4613747937\H,1.6284717846,-1.2590724514,-1.9504893882\H,1.5080133375,-3.0344502357,-2.0169354795\H,4.0724300705,-1.3737812081,-2.2228902813\H,3.2820736145,-2.2858728325,-3.5416215798\Zn,-2.2461693263,-0.7363727853,0.6306771595\Cl,-3.3809003539,-1.8561201278,-0.926967683\Cl,-2.1733944242,-1.0254541689,2.8244570084\O,-2.977051174,1.1288156926,0.1701882467\C,-3.9587511873,1.3918532346,-0.5290508418\C,-3.8126815851,1.8189237215,-1.9429370306\C,-2.4349751479,1.631950693,-2.5086890667\C,-4.8646499722,2.3052004624,-2.6064352112\O,-5.1870984341,1.3133180565,-0.0705922997\C,-5.3442595225,0.7795770681,1.2580600411\H,-1.6962652359,2.1992573628,-1.9352702084\H,-2.4040089219,1.9542491188,-3.5507229026\H,-2.1517302409,0.5752416826,-2.4512658778\H,-5.8371092431,2.3930957042,-2.1351300052\H,-4.768944114,2.6183448632,-3.6413336935\H,-6.3868616398,0.951420174,1.5142811339\H,-4.6726410399,1.2845529458,1.953145918\H,-5.1262640571,-0.2915092281,1.2398955589\\Version=ES64L-G09RevD.01\State=1-A\HF=-4232.5155673\RMSD=3.038e-09\RMSF=1.787e-06\Dipole=1.3661483,2.6645598,-0.6999359\Quadrupole=1.8484856,9.8216183,-11.670104,-13.5063214,8.1694685,-6.613309\PG=C01 [X(C20H29Cl2N1O4S1Zn1)]\\@

amine-bound [$ZnCl_2$(MMMP)(MMA)]

1\1\GINC-R3383\FOpt\RM062X\Gen\C20H29Cl2N1O4S1Zn1\ROOT\21-Feb-2016\0\\#M062X/gen 6D 10F INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=939524096\\MMMP_ZnCl2.Nmor.MMA.2b.freq\\0,1\C,-4.7079689053,-0.0551849154,-0.8453268116\C,-3.6019067454,-0.83162645,-1.1766837593\C,-2.4690389072,-0.8733662761,-0.3566819504\C,-2.4577192781,-0.0916238638,0.8089517611\C,-3.5451963952,0.7040794511,1.1305365046\C,-4.6889275789,0.7252101395,0.3155069274\C,-1.322373516,-1.6997982493,-0.8503449712\O,-1.1937765763,-1.8507634045,-2.0534770159\C,-0.3621226347,-2.5003132108,0.080623087\C,-0.4395247403,-3.9480605166,-0.4560337672\C,-0.8261320484,-2.5569569534,1.5417870259\N,1.046691683,-1.8960354638,-0.0229154093\S,-6.0073496835,1.7742403146,0.8365265663\C,-7.2186573441,1.5838573911,-0.4921048198\C,1.9251535234,-2.5074665236,1.0239010888\C,3.3802683575,-2.1006243408,0.8447271929\C,1.6543886179,-2.1633922484,-1.3670201087\C,3.1352141468,-1.8126938228,-1.4292557582\O,3.860043909,-2.4933279714,-0.4224129783\H,-5.5723163523,-0.0646205827,-1.4989172959\H,-3.6111841864,-1.4255366792,-2.085748939\H,-1.5881705003,-0.0451106073,1.4555400127\H,-3.5004942674,1.3290533009,2.018585382\H,-1.4276445076,-4.3438281633,-0.2022467597\H,0.3020629627,-4.5888879568,0.0268351022\H,-0.3280398713,-4.0042822484,-1.5370849891\H,-1.9084350065,-2.7051286304,1.5642406645\H,-0.5823876837,-1.6673573068,2.1200515247\H,-0.3717080702,-3.417686453,2.0390628684\H,-8.0510825529,2.2372963628,-0.2277124551\H,-7.5834963493,0.5568459316,-0.5551754169\H,-6.80896949,1.9042305848,-1.4521307017\H,1.8655727945,-3.6010738067,0.9644544918\H,1.5800110942,-2.1744342172,2.0045541271\H,3.9833853521,-2.615292105,1.5958852562\H,3.514781493,-1.016465815,0.9841946594\H,1.1025325951,-1.5970871679,-2.1193625795\H,1.5619185252,-3.2292723389,-1.5952264489\H,3.3053365835,-0.7334267544,-1.3514330693\H,3.524565666,-2.1573097577,-2.3901601443\Zn,1.1652910028,0.235060449,0.3844168343\Cl,2.8951023578,1.5195769306,-0.2821145218\Cl,0.6655945976,0.4550063775,2.5778458726\O,-0.170099534,0.9617766641,-0.994542534\C,-0.9312633481,1.9177379134,-1.1640898943\C,-1.2312238515,2.9928534375,-0.1866808048\C,-2.5300050162,3.7343923701,-0.3580320478\C,-0.3072149006,3.2949223405,0.7309619809\O,-1.5823171511,2.0665065893,-2.2996433062\C,-1.3021625258,1.1196217021,-3.3463524036\H,-3.3799659317,3.0472919864,-0.4069407012\H,-2.5234756834,4.3132201974,-1.2861471679\H,-2.6813274134,4.4169663816,0.4803494784\H,0.6594207579,2.805615427,0.782930381\H,-0.4896968233,4.0931323627,1.4442042582\H,-1.8966527344,1.4525936248,-4.1942535186\H,-1.5837961148,0.1148219859,-3.0304468916\H,-0.2369218007,1.1467645852,-3.5842531074\\Version=ES64L-G09RevD.01\State=1-A\HF=-4232.5218378\RMSD=7.464e-09\RMSF=6.077e-06\Dipole=-3.4867936,-1.038029,-1.5256875\Quadrupole=-3.8446071,6.5807996,-2.7361925,-12.3607406,4.8858521,-4.6981336\PG=C01 [X(C20H29Cl2N1O4S1Zn1)]\\@

thioether-bound [$ZnCl_2$(MMMP)(MMA)]

1\1\GINC-R2804\FOpt\RM062X\Gen\C20H29Cl2N1O4S1Zn1\ROOT\31-May-2016\0\\#M062X/gen 6D 10F INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=939524096\\MMMP_ZnCl2.S.MMA.2d.freq\\0,1\C,-0.8961307809,1.332391319,-2.0393018392\C,0.3468078109,1.8463522444,-1.6960784081\C,1.3423522873,1.0171542903,-1.1644270815\C,1.0600787145,-0.340255834,-0.9676073244\C,-0.1971320144,-0.8567355364,-1.2766894137\C,-1.1714852108,-0.0223750603,-1.8245626257\C,2.6481890236,1.6872734379,-0.8198943831\O,2.6559027496,2.8911790679,-0.6484827959\C,3.9743518886,0.8919298504,-0.7770588093\C,5.1258951684,1.8643587102,-0.4923051492\C,4.1589858837,0.2798127182,-2.1773792234\N,3.8332666748,-0.1743211115,0.2331099092\S,-2.8086621629,-0.5841923596,-2.2491730537\C,-2.5335213255,-2.3155478029,-2.7225310216\C,4.9199517874,-1.1508364892,0.2790353912\C,4.5325235466,-2.2832027782,1.2225097076\C,3.5702840485,0.321112972,1.5832160476\C,3.2028269005,-0.8518994059,2.4820210612\O,4.2502079497,-1.79

91879827,2.5199384695\H,-1.6483193649,1.9760873031,-2.4875500519\H,0.5682781616,2.897570014,-1.8511890373\H,1.8188255817,-0.9822967855,-0.5346883953\H,-0.4184540352,-1.8963197467,-1.0599720904\H,5.2160500462,2.5931945725,-1.3010021496\H,6.0668150942,1.3116324732,-0.4194250213\H,4.965285027,2.4242230261,0.430931771\H,3.9697622869,1.0399713928,-2.9413731921\H,3.4726236726,-0.554616631,-2.3427037911\H,5.185813435,-0.0695686045,-2.3138830098\H,-3.491421253,-2.6718865459,-3.1049857321\H,-2.2445911995,-2.9145770745,-1.8578422075\H,-1.7821666582,-2.3559503621,-3.5119407779\H,5.8650914627,-0.7020467977,0.6322988779\H,5.0864083446,-1.5690182379,-0.717255352\H,5.3540965379,-2.9955828439,1.3252554482\H,3.6503024937,-2.8078961936,0.8217818693\H,2.7401163072,1.0382253037,1.5541295144\H,4.4469101368,0.8346958218,2.0144073714\H,2.2811121758,-1.3298486437,2.1102010163\H,3.042569161,-0.5188818388,3.5106864891\Zn,-3.7193823089,-0.945154348,0.1171429464\Cl,-2.4708564747,-2.6347520287,0.8402018309\Cl,-5.8711259889,-0.5193974491,0.0415453734\O,-2.8552594385,0.7019652722,0.8727087666\C,-2.1366002922,1.6970290971,0.9073264389\C,-0.7900478056,1.722283303,1.5251585539\O,-2.5443343817,2.8511640888,0.4160491732\C,-3.8553929209,2.8463196939,-0.180405593\C,-0.3434007172,0.5529628389,1.9969827573\C,-0.0431479131,3.0238934045,1.5820673657\H,-4.0581150937,3.8826555611,-0.4387983885\H,-4.5905090521,2.4539018928,0.5238032323\H,-3.8543333067,2.216054684,-1.0742951484\H,-0.9345612117,-0.3564057154,1.9156146386\H,0.629168046,0.4898528998,2.4760530216\H,0.1550573784,3.4131859178,0.5794699313\H,0.9168957696,2.8834154816,2.0832904524\H,-0.6148946417,3.7819855547,2.1251136406\\Version=ES64L-G09RevD.01\State=1-A\HF=-4232.5127218\RMSD=5.342e-09\RMSF=6.546e-06\Dipole=2.781904,1.3825892,-1.7439267\Quadrupole=-14.6906607,4.4265323,10.2641284,-15.7796785,2.3108445,11.5562696\PG=C01 [X(C20H29Cl2N1O4S1Zn1)]\\@

ether-bound [$ZnCl_2$(MMMP)(MMA)]

1\1\GINC-R3304\Freq\RM062X\Gen\C20H29Cl2N1O4S1Zn1\ROOT\21-Feb-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/ChkBas Freq\\MMMP_ZnCl2.Omor.MMA.1b.freq\\0,1\C,6.4193373211,-0.9034380815,-0.7864540376\C,5.5035268144,0.1039562282,-1.0653209828\C,4.2901620457,0.2033223466,-0.3747647718\C,4.0166028681,-0.7473298678,0.6220442901\C,4.9290890367,-1.7516489072,0.9111494259\C,6.1404038766,-1.8455599754,0.2101464963\C,3.392825846,1.3473820014,-0.763419157\O,3.7753135507,2.1410410822,-1.6022996985\C,2.0223067446,1.5863485618,-0.082930178\C,1.265715702,2.6720573624,-0.8602573768\C,2.3307251398,2.1093668237,1.3330486562\N,1.299654437,0.3023358991,-0.0172014469\S,7.2147396085,-3.1713269186,0.6609571627\C,8.6251124781,-2.9391936807,-0.4459155493\C,0.0666008261,0.3058778579,0.7642955769\C,-0.4185691438,-1.1226499619,0.9318507824\C,1.0426591044,-0.2881535132,-1.3300985356\C,0.5550105723,-1.7132071009,-1.152862871\O,-0.6426560221,-1.7196304611,-0.3556584323\H,7.3447478052,-0.9433935885,-1.3490078477\H,5.7197629159,0.8391517331,-1.8335427856\H,3.0753819162,-0.713081938,1.1549930674\H,4.702282519,-2.4768060694,1.6877703113\H,1.8104000495,3.6170152885,-0.8192129381\H,0.2759722143,2.8205942866,-0.4185306912\H,1.1499097638,2.410580653,-1.9142066953\H,3.0851702094,2.8986376177,1.2714595296\H,2.7095107248,1.3204341736,1.9875258407\H,1.4371633558,2.5486107708,1.7853320166\H,9.3245364279,-3.7406944523,-0.2042411208\H,9.1144141821,-1.9790101207,-0.2713126697\H,8.3296322192,-3.0319650711,-1.4927885403\H,-0.7402022155,0.8950346422,0.2928083644\H,0.2530307962,0.7190393402,1.7590341079\H,-1.372790978,-1.1573223487,1.4591865274\H,0.3307499608,-1.7305576149,1.4537775244\H,1.9682115694,-0.3072475765,-1.9165830519\H,0.2864709473,0.2707647646,-1.9065832185\H,1.3058632483,-2.3235882919,-0.63639018\H,0.2900629859,-2.1631129397,-2.1111390305\Zn,-2.443045689,-1.3961822891,-1.298951763\Cl,-3.6859484288,-0.2890661578,0.1640662945\Cl,-1.9847972294,-0.9321948127,-3.4205273418\O,-2.9654272236,-3.3700571739,-1.2835065027\C,-3.7620396506,-4.2166887149,-1.6860257709\O,-4.9170308722,-3.9300262047,-2.2422814679\C,-5.2700460216,-2.5399832774,-2.3923532602\C,-3.4564646631,-5.6670577537,-1.557114534\C,-2.1287687368,-5.9849115466,-0.9320840095\C,-4.3378284136,-6.5750216518,-1.9849682846\H,-6.2666753665,-2.5480439763,-2.8270418829\H,-4.5639408165,-2.0500465113,-3.0677309073\H,-5.279792762,-2.0478318365,-1.4170544171\H,-2.0614503724,-5.5569209309,0.07194522\H,-1.3128642696,-5.5532043101,-1.5188907509\H,-1.9880069024,-7.0649856269,-0.8692800823\H,-5.2817792643,-6.2816393895,-2.4298127018\H,-4.1234647414,-7.6353607894,-1.8958357109\\Version=ES64L-G09RevD.01\State=1-A\HF=-4232.519947\RMSD=3.211e-09\RMSF=2.267e-06\ZeroPoint=0.4724381\Thermal=0.5065812\Dipole=0.887789,-2.7900663,0.8334507\PG=C01 [X(C20H29Cl2N1O4S1Zn1)]\\@

[$ZnCl_2$(DMPA)]

1\1\GINC-R162\Freq\RM062X\Gen\C16H16Cl2O3Zn1\ROOT\20-Jan-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/ChkBas Freq\\DMPA_ZnCl2.BI.freq\\0,1\O,0.7820161715,0.9318270626,-0.422492906\C,-0.3246020282,0.7288094934,0.0694223559\C,-1.3897367127,1.7440832994,-0.0593440378\C,-2.6667283948,1.5928906887,0.500478399\C,-3.6127705283,2.599794767,0.3401008986\C,-3.2946735771,3.7542179756,-0.3740436182\C,-2.0240261948,3.9096763187,-0.9309860614\C,-1.0737256436,2.9105686752,-0.773409346\C,-0.5841785804,-0.6187610225,0.8087149133\O,-1.1016302662,-0.4107029531,2.0781118527\O,0.6877216388,-1.2296605402,0.885267518\C,-1.5312355431,-1.4739158846,-0.0162992963\C,-2.7510024801,-1.9179296929,0.4900436673\C,-3.5711032382,-2.7226646202,-0.2997516304\C,-3.1728313159,-3.0799167494,-1.5866211653\C,-1.9453426093,-2.6423934152,-2.084337599\C,-1.1200082613,-1.841366036,-1.3007607498\C,-0.2616182695,0.3780379247,2.9295166221\C,0.7311091242,-2.5729985821,1.3849761667\H,-2.9175550043,0.7028779225,1.0627850477\H,-4.6002489237,2.4824181082,0.7733428784\H,-4.0381367784,4.5356606338,-0.4966958248\H,-1.7770242283,4.8089196841,-1.4850108749\H,-0.0804426724,3.0136035421,-1.1965139014\H,-3.0465090553,-1.6448008988,1.4978428537\H,-4.5195434192,-3.0738191845,0.0939213332\H,-3.8142667723,-3.7059700429,-2.1985956071\H,-1.6232964229,-2.9311165124,-3.0792986694\H,-0.1465353365,-1.5300456679,-1.6775424047\H,-0.7314869247,0.3615611266,3.9113929188\H,-0.2076215696,1.4127899633,2.5688637173\H,0.7484459391,-0.0382877435,2.9788161662\H,1.7633615162,-2.7408232147,1.6940123219\H,0.4528088801,-3.2721413615,0.5935134617\H,0.0623166423,-2.6670997165,2.2436267954\Zn,2.371813654,-0.3542149978,-0.0100716\Cl,3.4938768271,0.426642363,1.7009491902\Cl,2.7450503579,-1.7129507126,-1.6892137856\\Version=ES64L-G09RevD.01\State=1-A\HF=-354

4.2495044\RMSD=3.449e-09\RMSF=9.204e-06\ZeroPoint=0.2917056\Thermal=0.3144688\Dipole=-4.2667931,0.6062669,0.5264522\PG=C01 [X(C16H16Cl2O3Zn1)]\\@

ketone-bound [$ZnCl_2$(DMPA)(MMA)]

1\1\GINC-R618\Freq\RM062X\Gen\C21H24Cl2O5Zn1\ROOT\29-Feb-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RM062X/ChkBas Freq\\DMPA_ZnCl2.OAcyl.MMA.2c.freq\\0,1\O,0.3445596452,1.2401641327,0.0968066931\C,-0.8330101968,1.5730927898,-0.0143727623\C,-1.3176247848,2.2634097725,-1.2242610808\C,-2.6476395115,2.1906338727,-1.6582781888\C,-3.0152857524,2.8173086846,-2.8436923383\C,-2.0728134935,3.5334931193,-3.5815524788\C,-0.7525182553,3.624996701,-3.1398223022\C,-0.3714920409,2.9854512293,-1.9679242731\C,-1.7891281061,1.175271007,1.1349822366\O,-2.8242713437,2.0983941541,1.2959968136\O,-0.9791608764,1.0924123965,2.2742421636\C,-2.3901364172,-0.1777319458,0.7568309848\C,-3.7710036602,-0.3740061382,0.7143650943\C,-4.2809078064,-1.6307704769,0.3935414597\C,-3.4161852935,-2.6865615706,0.1090897226\C,-2.0373287698,-2.4879289049,0.1544096362\C,-1.5214042461,-1.2371142659,0.4805004502\C,-2.3995185958,3.3904166795,1.7106168172\C,-1.6370628155,0.5795555063,3.4252779359\H,-3.3771498366,1.6247865758,-1.0916640237\H,-4.0382375174,2.740689869,-3.196633634\H,-2.3680327209,4.0205125488,-4.5057295779\H,-0.0192835485,4.1832402271,-3.7117000169\H,0.6549942775,3.0570890068,-1.6154020162\H,-4.4357100097,0.4536139602,0.9378345095\H,-5.355201503,-1.7830838165,0.3632994142\H,-3.8163355943,-3.6609353763,-0.1527873676\H,-1.3578644837,-3.2999693538,-0.0816519877\H,-0.444502096,-1.0901408884,0.5161386149\H,-3.2859440227,4.0234850082,1.6834191025\H,-1.6438600441,3.7997510419,1.0284246879\H,-1.9884871953,3.3623854623,2.7239286631\H,-0.9424666263,0.7192943069,4.2541662511\H,-1.8625606407,-0.4852846524,3.3064577601\H,-2.565372905,1.1260151729,3.6258778219\Zn,1.5914048613,0.3874503481,-1.3156727376\Cl,3.385427475,1.6651544488,-1.5914255838\Cl,0.2561321159,-0.6605716644,-2.7167363761\O,2.1761401538,-0.9397063796,0.1235755222\C,3.1773917176,-1.0029073747,0.8410345707\C,3.2155473824,-0.5533854194,2.2537659238\O,4.3139770944,-1.5024669988,0.4075271538\C,4.3624387151,-1.8970184286,-0.9776164162\C,4.4537243778,-0.8380140209,3.0557783731\C,2.1446845858,0.1167029096,2.6928695374\H,5.3055854778,-2.4262107723,-1.0903518942\H,4.3417979008,-1.001921539,-1.6034580916\H,3.5142130496,-2.5424264 1,-1.2104552004\H,5.3270216047,-0.3611978847,2.6022084114\H,4.6579364518,-1.911648097,3.0998184646\H,4.3360872151,-0.4610129396,4.073246365\H,1.2931195145,0.3211539803,2.0486936835\H,2.1182394909,0.4963684067,3.7105598101\\Version=ES64L-G09RevD.01\State=1-A\HF=-3889.9108239\RMSD=9.941e-10\RMSF=2.368e-06\ZeroPoint=0.4176235\Thermal=0.4500387\Dipole=-1.401802,-0.011538,2.296865\PG=C01 [X(C21H24Cl2O5Zn1)]\\@

[$AlCl_2$(MMMP)]$^+$

1\1\GINC-R48\FOpt\RM062X\6-31+G(d,p)\C15H21Al1Cl2N1O2S1(1+)\ROOT\28-Jul-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=2013265920\\CAT5.freq\\1,1\C,-0.029466793,0.1850860848,-0.0502520845\C,-0.0678124591,0.0268916664,1.3201355514\C,1.1099650616,-0.2094925802,2.0654037445\C,2.3422824613,-0.2505397655,1.3713896516\C,2.3860935509,-0.0737898395,0.0077201038\C,1.2007300913,0.1378921194,-0.7334032692\C,0.9600351264,-0.3596543432,3.4926658991\O,-0.1398212992,-0.048062729,4.0137995683\C,2.0557436475,-0.8154955461,4.4819831617\C,2.8531924725,0.4663621803,4.7995590754\C,3.0011416484,-1.9173559245,3.9850031036\N,1.2843978431,-1.2838362555,5.6941285828\S,1.3865636385,0.3282322873,-2.4504251457\C,-0.3039145722,0.6023217682,-3.0323069062\C,1.9816561842,-1.1497109129,7.0019208605\C,0.8926153512,-1.2988154331,8.0962712078\C,0.7941298319,-2.6931458616,5.5813181366\C,-0.1678426541,-2.9210420686,6.7798754957\O,-0.3366225138,-1.6423940725,7.4292811037\H,-0.955903083,0.3480732812,-0.5868728662\H,-1.0184810082,0.067805288,1.8410185859\H,3.2797938147,-0.3821858026,1.8941253056\H,3.3413269614,-0.0893473878,-0.5075222549\H,3.2058214464,0.9070642507,3.8645927865\H,3.7325699514,0.2298885162,5.4038254847\H,2.2379613456,1.2107055154,5.3128639111\H,3.8023801611,-1.5046260054,3.3752234646\H,2.4922444205,-2.6915125194,3.4058213343\H,3.4878091691,-2.3838051674,4.8471228053\H,-0.2185164891,0.7321796455,-4.1117475628\H,-0.7281863448,1.5102321118,-2.6007355948\H,-0.9376406406,-0.2627237479,-2.8306364836\H,2.4327437707,-0.1629877077,7.0765220292\H,2.7645798357,-1.9120616158,7.0904444357\H,0.7050034052,-0.3603825838,8.6143375271\H,1.1253404735,-2.0823066061,8.8201952421\H,1.6291440245,-3.3987809244,5.602029603\H,0.2647349436,-2.80470761,4.6287044207\H,0.236774344,-3.6244402191,7.5103883638\H,-1.1569102724,-3.2453853317,6.4625465956\Al,-0.5563771518,-0.3346251503,5.8348021288\Cl,-0.1930567105,1.5089389277,6.794372835\Cl,-2.4858483281,-1.1091908465,5.4291058416\\Version=ES64L-G09RevD.01\State=1-A\HF=-2350.0255916\RMSD=4.026e-09\RMSF=5.323e-06\Dipole=2.5560606,-1.9060702,-0.1947332\Quadrupole=-17.5706097,-16.8194926,34.3901023,-1.9507907,15.5602257,-20.3493963\PG=C01 [X(C15H21Al1Cl2N1O2S1)]\\@

[$AlCl_2$(MMMP)][$AlCl_4$]

1\1\GINC-R44\FOpt\RM062X\6-31+G(d,p)\C15H21Al2Cl6N1O2S1\ROOT\30-Jul-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=1610612736\\CAT5.AlCl4.3.freq\\0,1\C,3.4482170421,-0.5597983457,-0.7775484958\C,2.111186115,-0.6024012297,-0.4229885539\C,1.5267798269,-1.78189534,0.0759947459\C,2.343365028,-2.9199969113,0.2339831299\C,3.6817805202,-2.8746291893,-0.0978759993\C,4.2550723705,-1.697644461,-0.6187593161\C,0.1092448907,-1.7218458295,0.4112013063\O,-0.4148799267,-0.5932828384,0.5205571378\C,-0.8027105935,-2.9310173523,0.6870553216\C,-0.5598369503,-3.2781481939,2.1711222158\C,-0.

548512696,-4.1587093406,-0.1949133013\N,-2.1938248668,-2.3925655673,0.4865406026\S,5.9551700821,-1.7710380368,-1.0224813856\C,6.3049351567,-0.1064630004,-1.6364232204\C,-3.2828818172,-3.0476465781,1.2729303392\C,-4.4790702111,-2.0624859048,1.247466704\C,-2.6351034618,-2.408569396,-0.9502114093\C,-3.9671554203,-1.6137824962,-1.0023233699\O,-4.1405979736,-1.0084223195,0.3143334329\H,3.8560676934,0.3611930831,-1.1755027534\H,1.4907510566,0.2794032226,-0.5440561256\H,1.9512828995,-3.8403781724,0.6448971172\H,4.3009636116,-3.7549875642,0.0435126654\H,0.5087348318,-3.427720695,2.3398176948\H,-1.068687846,-4.2122866421,2.4207069432\H,-0.9005149436,-2.4784209481,2.8348792068\H,0.2915783219,-4.7435217728,0.175958566\H,-0.3572367058,-3.9014291977,-1.2396441108\H,-1.4256669308,-4.8098536837,-0.1618961127\H,7.3630116407,-0.1110633653,-1.9008165709\H,6.1378319181,0.6453881839,-0.8632135216\H,5.7194310469,0.1180259409,-2.5296777283\H,-2.9591300754,-3.1946506234,2.3008959831\H,-3.5393714839,-4.0139416753,0.8214126637\H,-4.6312425668,-1.5741114538,2.2081866814\H,-5.3955886448,-2.5440072263,0.9070288012\H,-2.7725472176,-3.4330873064,-1.3022255766\H,-1.8643601876,-1.9257369452,-1.562182057\H,-4.8247354747,-2.2586547228,-1.1955183961\H,-3.9392364426,-0.7982369151,-1.7217086826\Al,-2.3015126588,-0.3698659398,0.7868916803\Cl,-2.4371282427,-0.0376478945,2.8789978014\Cl,-2.3937355702,1.2421705071,-0.6019290282\Al,-5.0786811479,-5.4533677276,-2.1391199306\Cl,-6.1198168008,-6.9922180242,-3.1480130473\Cl,-6.2981102931,-4.460950115,-0.6443139933\Cl,-4.3482183955,-3.9175337569,-3.4783542464\Cl,-3.3543285067,-6.2096562391,-1.0519838071\\Version=ES64L-G09RevD.01\State=1-A\HF=-4433.6079963\RMSD=2.329e-09\RMSF=4.243e-06\Dipole=6.6457918,2.5241,2.2985933\Quadrupole=21.9365984,-20.4311986,-1.5053998,-9.6728092,-20.800717,-22.8537747\PG=C01 [X(C15H21Al2Cl6N1O2S1)]\\@

ketone-amine bound $[AlCl_2(MMMP)]^+$

1\1\GINC-R38\FOpt\RM062X\6-31+G(d,p)\C15H21Al1Cl2N1O2S1(1+)\ROOT\29-Jul-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=2013265920\\CAT1.freq\\1,1\C,-0.0293388438,-0.1354299199,-0.024629275\C,0.0131997092,-0.2075949474,1.3499051123\C,1.22608902,-0.0293608691,2.0636591242\C,2.4099700415,0.1967355827,1.3146493249\C,2.3739605064,0.2481099705,-0.0572742833\C,1.1531465667,0.0941328123,-0.7584356077\C,1.1601687937,-0.1316208037,3.4910563534\O,0.0825275303,-0.5697208413,4.0051898639\C,2.2881603937,0.1506092703,4.5046980578\C,3.2928375298,1.2409724866,4.1029882876\C,3.038314714,-1.195363564,4.6362821902\N,1.5689826384,0.5091000438,5.826381456\S,1.2381166252,0.1986027352,-2.484479206\C,-0.4713432332,-0.0603300144,-3.0164140917\C,2.454210099,0.2536784668,7.0145222534\C,1.8106188466,0.7795101862,8.2891574336\C,1.158538334,1.9665264192,5.8277936304\C,0.6378021014,2.4288934353,7.1894268164\O,1.5886596576,2.1650665515,8.1944398084\H,-0.9792290217,-0.2600362943,-0.5294493648\H,-0.9007367989,-0.3888052086,1.9043050362\H,3.3706992577,0.2980415742,1.7978989536\H,3.2921032933,0.4037457596,-0.6148230363\H,4.0887480055,0.8105152459,3.4971877157\H,3.7848943126,1.6390750252,4.9931160013\H,2.8410435036,2.0693668814,3.5539187998\H,3.3628934238,-1.5109020578,3.6415294453\H,2.4176672005,-1.9888635389,5.0583026856\H,3.9319829224,-1.0695984077,5.251342298\H,-0.4444854603,-0.0010456334,-4.1050123057\H,-1.1266925331,0.7250594463,-2.6368089745\H,-0.8296422146,-1.0490509742,-2.7258928533\H,3.4099740113,0.7673252888,6.8660198088\H,2.6236722075,-0.8200511837,7.1009595823\H,2.4881182654,0.6077810147,9.1271820443\H,0.8658826586,0.2493048455,8.5018017531\H,0.4002443511,2.1160775033,5.0503538952\H,2.0320240724,2.5753334172,5.5930887337\H,-0.3209293026,1.9652611591,7.4455713086\H,0.4949643215,3.5103720678,7.147676544\Al,-0.1009965139,-0.6179002262,5.8174266066\Cl,0.3305549983,-2.4526462601,6.7272640744\Cl,-1.928941695,0.2977311074,6.2419128752\\Version=ES64L-G09RevD.01\State=1-A\HF=-2350.0170015\RMSD=2.451e-09\RMSF=5.426e-06\Dipole=1.648066,0.7607751,-2.2225833\Quadrupole=-9.2990557,-21.2209537,30.5200093,-0.8348857,15.0090824,3.503025\PG=C01 [X(C15H21Al1Cl2N1O2S1)]\\@

$[AlCl_2(DMPA)]^+$

1\1\GINC-R78\FOpt\RM062X\6-31+G(d,p)\C16H16Al1Cl2O3(1+)\ROOT\28-Jul-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=2013265920\\DMPA_AlCl2+.freq\\1,1\O,0.0953272448,0.0106614498,-0.0086008198\C,0.0908668324,0.001798515,1.2517051026\C,1.3209314384,0.0036843807,1.9942518861\C,1.3391834101,-0.0100403691,3.4064897965\C,2.5549317386,-0.0223449975,4.0704601104\C,3.7486956677,-0.0166125294,3.342826604\C,3.7389131239,-0.0015531046,1.9440063803\C,2.5322824794,0.0074330132,1.2669899608\C,-1.2989670668,0.0041058754,1.946546221\O,-1.467055132,-1.0412280756,2.806250822\O,-2.2267428281,-0.1416613485,0.8124359868\C,-1.5578007647,1.3275848976,2.6330518276\C,-1.9856267515,1.3687278204,3.959916374\C,-2.2423932938,2.6025870974,4.55534834\C,-2.0713064849,3.7813306385,3.8312008649\C,-1.6460988155,3.7338996717,2.5031796297\C,-1.3881751403,2.5066074181,1.9009048412\C,-1.2365999957,-2.3538061159,2.2680415804\C,-3.6459318899,-0.0360116257,1.1220901355\H,0.4144383278,-0.0112511806,3.9711425212\H,2.5789462418,-0.0326559548,5.1541813983\H,4.6969795138,-0.0231619853,3.8711470482\H,4.6721040213,0.0028520035,1.3923206216\H,2.5042387173,0.016864126,0.1828543966\H,-2.1203179153,0.447525156,4.5168465522\H,-2.5798491213,2.6406395642,5.5855671674\H,-2.2719274367,4.7387219791,4.3003096351\H,-1.5169155611,4.6494052253,1.9363628528\H,-1.07125788,2.4794520032,0.8595852928\H,-1.4250152078,-3.0438817157,3.0873942101\H,-0.198518886,-2.45997046,1.9332970451\H,-1.9208541635,-2.5582263215,1.4400120455\H,-3.9074715286,1.0177488015,1.2187261715\H,-3.8312988434,-0.5833629428,2.0462520835\H,-4.1721725938,-0.5036522461,0.2897703154\Al,-1.5033703004,-0.1413332485,-0.9150553971\Cl,-1.7601333432,-2.0405806873,-1.7105981791\Cl,-2.0465350401,1.6157703015,-1.8738155638\\Version=ES64L-G09RevD.01\State=1-A\HF=-2007.405172\RMSD=5.972e-09\RMSF=1.109e-05\Dipole=0.862271,-0.1635307,2.3769511\Quadrupole=14.3401824,-7.1623262,-7.1778561,-2.9744433,2.4078644,1.8749296\PG=C01 [X(C16H16Al1Cl2O3)]\\@

$[AlCl_2(DMPA)(MMA)]^+$

1\1\GINC-R65\FOpt\RM062X\6-31+G(d,p)\C21H24Al1Cl2O5(1+)\ROOT\02-Aug-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=2013265920\\DMPA_AlCl2+.MMA.1.freq\\1,1\O,-0.5860312124,0.1372885691,-0.1676233673\C,-0.2985485287,0.1046898824,1.0514872681\C,1.0822157837,0.147335016,1.48443209\C,1.4387420244,0.0537165333,2.8441927098\C,2.7788

456075,0.0896815974,3.202879875\C,3.7624332656,0.2255289748,2.2215803375\C,3.4153422638,0.3235575994,0.8702922224\C,2.0819541108,0.2822148831,0.5001922768\C,-1.4806423301,0.0301546546,2.0478999404\O,-1.376163035,-1.0520996162,2.8923155755\O,-2.6057802065,-0.1143283251,1.1735025595\C,-1.578681184,1.3139913032,2.8531466346\C,-1.6419714496,1.2807886748,4.2459419277\C,-1.7548648756,2.4753786465,4.9552951775\C,-1.8009533004,3.6928327521,4.2782147502\C,-1.7412226757,3.7206031631,2.8851642444\C,-1.6305189392,2.5317973169,2.1699784208\C,-1.3045572528,-2.3351804753,2.2579971601\C,-3.9086770225,-0.0693451393,1.8030614503\H,0.6765769872,-0.051121943,3.6065778522\H,3.0593129074,0.015995527,4.2475076363\H,4.8081978776,0.2579225347,2.510565282\H,4.1875087915,0.4335289472,0.1170814599\H,1.7908297129,0.3618239209,-0.5412520611\H,-1.6112829076,0.3301630072,4.7674268478\H,-1.8111608989,2.4523793285,6.0384594471\H,-1.8885690081,4.6198456505,4.835083874\H,-1.7861583851,4.6652927826,2.3541933144\H,-1.6125758094,2.5604331529,1.0827070263\H,-1.2312765644,-3.0596334765,3.0665710389\H,-0.4111115784,-2.4081450217,1.6250550305\H,-2.1977398141,-2.523746527,1.6570536575\H,-4.18250543,0.9709322065,1.98287269\H,-3.8631539471,-0.6385871171,2.7325128955\H,-4.5959921505,-0.5407496539,1.1017905607\Al,-2.3535060263,-0.0268645402,-0.8241932541\Cl,-3.1429880602,-2.0081197743,-1.0254212017\Cl,-3.4786990314,1.7762429046,-0.948975753\O,-1.5660075482,0.0209080589,-2.536359776\C,-1.6243894287,-0.3680033655,-3.7206510257\O,-0.513493508,-0.5908594298,-4.3696570742\C,-2.8734253702,-0.572684629,-4.4807885031\C,-2.8050866061,-1.2761624243,-5.6187793011\C,-4.1376541466,0.0185025287,-3.9243267386\H,-3.7020380082,-1.4588006281,-6.2016852723\H,-1.8719464771,-1.6884421943,-5.9851794933\C,0.7255018192,-0.4522618854,-3.6511864865\H,1.4995268615,-0.7025672739,-4.3717734106\H,0.8308338084,0.5762518846,-3.3028868747\H,0.7375767558,-1.1419896662,-2.8053892226\H,-4.945613986,-0.1101485297,-4.6456663399\H,-4.4340901734,-0.4740135617,-2.9940376088\H,-4.0209417008,1.085018196,-3.7164854685\\Version=ES64L-G09RevD.01\State=1-A\HF=-2353.1089024\RMSD=5.264e-09\RMSF=1.673e-06\Dipole=2.2959333,-0.4128885,0.0461137\Quadrupole=0.4615359,-25.5913174,25.1297814,-0.5799571,5.3690874,10.3718064\PG=C01 [X(C21H24Al1Cl2O5)]\\@

$[AlCl_2(MMA)_2]^+$

1\1\GINC-R111\FOpt\RM062X\6-31+G(d,p)\C10H16Al1Cl2O4(1+)\ROOT\07-Feb-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=134217728\\AlCl2+mon2.2.freq\\1,1\Cl,-0.133683271,-2.6009848935,0.5234293939\Al,-0.0890083201,-0.6579550757,-0.2656006917\Cl,-0.422799535,-0.346313908,-2.3099284044\O,-1.2163420463,0.4069952352,0.6805731243\C,-2.3951367016,0.8583738917,0.6448914028\C,-3.5331199357,0.2595918212,-0.0698925052\C,-3.46501687,-1.0384336686,-0.393788566\C,-4.7254108195,1.1419197209,-0.3223422373\O,-2.6677817164,1.9476582519,1.2868258129\C,-1.6175820219,2.6157183114,2.0231411978\H,-2.6226459127,-1.6747460139,-0.1394505098\H,-4.2965718592,-1.5185886894,-0.8994447502\H,-4.4439596892,2.0353284719,-0.8858588279\H,-5.1730386936,1.4703581571,0.6191346531\H,-5.4750281428,0.5928677342,-0.892286324\H,-2.0918158899,3.4956331674,2.4480763223\H,-0.8150988113,2.8914063172,1.3385337411\H,-1.2466781184,1.9516040958,2.8038147001\O,1.4637738362,0.1107170570,0.2240816443\C,2.7092333378,0.2956176372,0.1517705112\C,3.3630757878,1.1654593237,-0.8365575446\O,3.5031549867,-0.2696000655,0.9987420616\C,2.9613867752,-1.168189324,1.999587272\C,4.8602965935,1.2869722849,-0.7722596693\C,2.5789707117,1.7793138837,-1.733737115\H,3.8147770641,-1.4498499434,2.609441167\H,2.522960202,-2.0355381872,1.5059479845\H,2.2101797732,-0.6419229862,2.5890840726\H,5.1821274869,1.6859706307,0.1931586202\H,5.21107413,1.954011048,-1.5598798144\H,5.3389071615,0.3127650064,-0.9014582239\H,1.5018825696,1.6509884078,-1.7458353133\H,3.0137979381,2.4221402999,-2.4922701847\\Version=ES64L-G09RevD.01\State=1-A\HF=-1854.0515922\RMSD=3.079e-09\RMSF=3.323e-06\Dipole=0.4309601,1.8611249,1.3808837\Quadrupole=23.8963621,-11.3500079,-12.5463543,-1.2732115,-0.1779103,0.0362573\PG=C01 [X(C10H16Al1Cl2O4)]\\@

$[AlCl_3(MMA)_3]^+$

1\1\GINC-R37\FOpt\RM062X\6-31+G(d,p)\C15H24Al1Cl2O6(1+)\ROOT\03-Aug-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=4831838208\\AlCl2mon3+.1.freq\\1,1\Al,-0.2807814131,0.4219582818,0.0776741221\O,-2.1237454898,-0.019269561,-0.201937243\O,-0.0192978748,-1.3944077198,0.2207613125\O,1.6547152552,0.6063110619,0.3681556025\Cl,-0.7339349372,1.3625558436,1.9651447854\Cl,-0.0162325332,1.1494928359,-1.9318057309\C,0.7168955501,-2.3836828073,0.4100887613\O,1.2686841874,-2.6208546643,1.5609220785\C,1.0289060545,-1.6987100963,2.6520716285\C,0.9522798452,-3.3529075382,-0.6785133873\C,1.6854791535,-4.4447452661,-0.4281127803\C,0.3306495399,-3.0058404383,-2.0022267213\C,2.658174853,1.1955099271,-0.0861861943\C,3.8060881591,0.4282012271,-0.6159355888\C,3.5976224616,-1.0542871951,-0.7287716714\C,4.9251528385,1.072337563,-0.9653463429\O,2.7771384881,2.4886381425,-0.1057442835\C,1.7318615393,3.314851586,0.449629253\C,-3.3136082266,0.3136189064,-0.0586289319\C,-3.814471775,1.7038408085,-0.1049030103\C,-2.8911633204,2.7607118276,-0.6416437659\C,-5.0572239036,1.9415801857,0.3332704833\O,-4.2195366693,-0.6125914549,0.1227084714\C,-3.7722779665,-1.9751952921,0.2283232108\H,1.5093943378,-2.1549786576,3.5130834756\H,-0.0446167783,-1.5897646071,2.8116875\H,1.4735331955,-0.7316434884,2.4148793302\H,2.1055219566,-4.6376497254,0.5531236317\H,1.8754692106,-5.1710536386,-1.2118584144\H,0.6627630988,-2.0233680582,-2.3537814244\H,-0.7592552957,-2.9593317081,-1.9217122378\H,0.5940971393,-3.7546682269,-2.749603616\H,2.7387899693,-1.2694972306,-1.3740020835\H,3.4064318793,-1.5018870923,0.2522193908\H,4.4782608712,-1.5323056286,-1.1595827351\H,5.0164998595,2.1480928918,-0.8667905394\H,5.7753261256,0.525894949,-1.3608531874\H,2.1479233595,4.3188370382,0.463989127\H,1.4830583987,2.9715625956,1.4535894616\H,0.8580243539,3.273373205,-0.2033552256\H,-2.512868599,2.4932332347,-1.6313316807\H,-2.0331221735,2.907903825,0.021391121\H,-3.4263903822,3.7083143017,-0.715208467\H,-5.6931116765,1.1507028641,0.7139428996\H,-5.4565827915,2.9505837922,0.3226274562\H,-4.6736222573,-2.5578497082,0.3990259005\H,-3.0792375979,-2.0702962556,1.06599401\H,-3.2836940195,-2.2728518353,-0.7003147503\\Version=ES64L-G09RevD.01\State=1-A\HF=-2199.7392929\RMSD=5.774e-09\RMSF=3.540e-06\Dipole=0.5047331,-1.6019551,0.4652264\Quadrupole=19.7992581,7.1695533,-26.9688114,-2.8601648,-2.2453674,0.5916354\PG=C01 [X(C15H24Al1Cl2O6)]\\@

9.5 BDE and Rate Coefficient Section

CH_3 rad

1\1\GINC-R3034\FOpt\UM062X\6-31+G(d,p)\C1H3(2)\ROOT\08-Jan-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=134217728\\CH3_rad.freq\\0,2\C,0.,0.,0.\H,0.5399863489,-0.9352837917,0.\H,0.5399863489,0.9352837917,0.\H,-1.0799726978,0.,0.\\Version=ES64L-G09RevD.01\State=2-A2"\HF=-39.8118974\S2=0.754807\S2-1=0.\S2A=0.750016\RMSD=6.428e-09\RMSF=1.252e-06\Dipole=0.,0.,0.\Quadrupole=0.5084417,0.5084417,-1.0168835,0.,0.,0.\PG=D03H [O(C1),3C2(H1)]\\@

CH_3rad-H

1\1\GINC-R3034\FOpt\RM062X\6-31+G(d,p)\C1H4\ROOT\08-Jan-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=134217728\\CH3_radH.freq\\0,1\C,0.1784749644,-0.0077513941,0.0186390444\H,0.256897066,-0.9090103818,-0.5905744126\H,0.2560453395,0.8717858216,-0.6216360081\H,-0.7831905385,0.0007660164,0.533112429\H,0.9841831686,0.005439938,0.7536289473\\Version=ES64L-G09RevD.01\HF=-40.487944\RMSD=6.378e-09\RMSF=9.771e-07\Dipole=0.0000075,-0.0000037,-0.0000031\Quadrupole=0.000084,0.0000277,-0.0001117,-0.000021,-0.0000054,-0.0000095\PG=D02D [O(C1),2SGD(H2)]\\@

B rad

1\1\GINC-R43\FOpt\UM062X\6-31+G(d,p)\C7H5O1(2)\ROOT\20-Jan-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\Acyl_rad.CS.freq\\0,2\O,0.,-0.2693847627,2.8497914316\C,0.,0.5120548974,1.9591436292\C,0.,0.2311726004,0.4988393105\C,0.,1.3004687249,-0.3972200134\C,0.,1.0505263968,-1.7673390566\C,0.,-0.2645514441,-2.2305635612\C,0.,-1.3346635651,-1.3317631281\C,0.,-1.091375528,0.0365756628\H,0.,2.3148517513,-0.0097491626\H,0.,1.8760461167,-2.4712928547\H,0.,-0.459463582,-3.2985450631\H,0.,-2.3548581784,-1.7019132887\H,0.,-1.9050234271,0.7554260944\\Version=ES64L-G09RevD.01\State=2-A'\HF=-344.7872236\S2=0.753727\S2-1=0.\S2A=0.750009\RMSD=8.023e-09\RMSF=5.529e-05\Dipole=0.,-0.0188185,-1.4050994\Quadrupole=-1.5982539,4.3545758,-2.7563219,0.,0.,0.1103\PG=CS [SG(C7H5O1)]\\@

B cation

1\1\GINC-R66\FOpt\RM062X\6-31+G(d,p)\C7H5O1(1+)\ROOT\23-Mar-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\B_cat.C2V.freq\\1,1\O,0.,0.,3.00313\C,0.,0.,1.87581\C,0.,0.,0.48373\C,0.,1.24493,-0.1911\C,0.,1.22354,-1.57326\C,0.,0.,-2.25497\C,0.,-1.22354,-1.57326\C,0.,-1.24493,-0.1911\H,0.,2.17828,0.3618\H,0.,2.15672,-2.12476\H,0.,0.,-3.34054\H,0.,-2.15672,-2.12476\H,0.,-2.17828,0.3618\\Version=ES64L-G09RevD.01\State=1-A1\HF=-344.5476602\RMSD=2.469e-09\RMSF=3.752e-05\Dipole=0.,0.,0.0421734\Quadrupole=-9.2198296,1.8761747,7.3436549,0.,0.,0.\PG=C02V [C2(H1C1C1C1O1),SGV(C4H4)]\\@

B rad $AlCl_3$

1\1\GINC-R56\FOpt\UM062X\6-31+G(d,p)\C7H5Al1Cl3O1(2)\ROOT\20-Jan-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\Acyl_rad_AlCl3.CS.freq\\0,2\O,0.,-0.34758,0.01203\C,0.,0.42847,-0.91734\C,0.,0.15521,-2.33582\C,0.,1.23636,-3.22685\C,0.,0.98715,-4.59374\C,0.,-0.33013,-5.05431\C,0.,-1.40807,-4.16234\C,0.,-1.17406,-2.79586\H,0.,2.24885,-2.83537\H,0.,1.81145,-5.29804\H,0.,-0.52277,-6.12262\H,0.,-2.42513,-4.53889\H,0.,-1.98992,-2.08001\Al,0.,-0.00548,1.92383\Cl,0.,2.10985,1.95868\Cl,1.79671,-0.94413,2.49351\Cl,-1.79671,-0.94413,2.49351\\Version=ES64L-G09RevD.01\State=2-A'\HF=-1967.9304399\S2=0.754734\S2-1=0.\S2A=0.750015\RMSD=2.536e-09\RMSF=2.274e-05\Dipole=0.,-0.079001,-4.3275176\Quadrupole=-8.8756262,-1.2667103,10.1423365,0.,0.,0.7473663\PG=CS [SG(C7H5Al1Cl1O1),X(Cl2)]\\@

B cation $AlCl_3$

1\1\GINC-R42\FOpt\RM062X\6-31+G(d,p)\C7H5Al1Cl3O1(1+)\ROOT\24-Mar-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT(calcfc) IOP(2/17=4) Freq=noraman maxdisk=402653184\\B_cat_AlCl3.freq\\1,1\O,-0.6737581531,-0.0552820083,-2.6822036202\C,-1.2858633958,-0.0409617904,-1.735866088\C,-2.0905387371,-0.0244311386,-0.5970822848\C,-2.4766551814,-1.2601144979,-0.0279672546\C,-3.299004777,-1.2237334009,1.0833090901\C,-3.7159446674,0.0067512769,1.605456666\C,-3.3220431582,1.2217388306,1.031672192\C,-2.5001032067,1.2266731837,-0.0804852953\H,-2.131319229,-2.1978191306,-0.4500339863\H,-3.6161988434,-2.1504599252,1.5474744769\H,-4.3607845901,0.0191168535,2.4786477214\H,-3.6568157217,2.161088133,1.4564474073\H,-2.1723315605,2.152068374,-0.5418857515\Al,2.1448539337,0.0320143719,0.1671616336\Cl,1.097540145,-1.7297836509,-0.2456071949\Cl,1.0650936365,1.7548266215,-0.3197969212\Cl,4.0158975061,0.0669048975,0.9941922095\\Version=ES64L-G09RevD.01\State=1-A\HF=-1967.6621559\RMSD=2.273e-09\RMSF=3.353e-06\Dipole=-3.514867,-0.0357433,-0.1144398\Quadrupole=12.6754164,-8.3549772,-4.3204391,0.0619157,-6.5512712,0.02465\PG=C01 [X(C7H5Al1Cl3O1)]\\@

B rad-H

1\1\GINC-R39\FOpt\RM062X\6-31+G(d,p)\C7H6O1\ROOT\20-Jan-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\Acyl_radH.CS.freq\\0,1\O,0.,-0.35066,-2.80077\C,0.,0.50366,-1.94432\C,0.,0.2271,-0.4869\C,0.,1.29389,0.41364\C,0.,1.04794,1.7848\C,0.,-0.26654,2.24898\C,0.,-1.33564,1.34828\C,0.,-1.09148,-0.01957\H,0.,2.31446,0.0374\H,0.,1.87448,2.48782\H,0.,-0.46111,3.31704\H,0.,-2.35577,1.71858\H,0.,-1.90086,-0.74334\H,0.,1.57937,-2.21915\\Version=ES64L-G09RevD.01\State=1-A'\HF=-345.4390913\RMSD=5.244e-09\RMSF=1.073e-04\Dipole=0.,0.5039109,1.2315373\Quadrupole=-1.8952427,4.9683935,-3.0731509,0.,0.,-2.9115266\PG=CS [SG(C7H6O1)]\\@

B rad-H $AlCl_3$

1\1\GINC-R56\FOpt\RM062X\6-31+G(d,p)\C7H6Al1Cl3O1\ROOT\20-Jan-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\Acyl_radH_AlCl3.CS.freq\\0,1\O,0.,-0.27495,0.00478\C,0.,0.57719,0.90727\C,0.,0.21614,2.30748\C,0.,1.24356,3.26187\C,0.,0.92343,4.61403\C,0.,-0.41677,5.00236\C,0.,-1.44326,4.05105\C,0.,-1.13259,2.70037\H,0.,2.28128,2.93894\H,0.,1.70887,5.36151\H,0.,-0.66734,6.05862\H,0.,-2.4793,4.3713\H,0.,-1.90673,1.93974\H,0.,1.64097,0.63111\Al,0.,-0.03712,-1.87502\Cl,-1.79939,-0.97139,-2.45264\Cl,1.79939,-0.97139,-2.45264\Cl,0.,2.08961,-2.01494\\Version=ES64L-G09RevD.01\State=1-A'\HF=-1968.601213\RMSD=3.054e-09\RMSF=1.695e-05\Dipole=0.,0.3310797,4.3543507\Quadrupole=-8.5982555,0.2402164,8.3580391,0.,0.,-0.3239218\PG=CS [SG(C7H6Al1Cl1O1),X(Cl2)]\\@

T rad

1\1\GINC-R1179\FOpt\UM062X\6-31+G(d,p)\C8H7O1S1(2)\ROOT\15-Feb-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\T_rad.1.freq\\0,2\O,-0.140434367,-0.0001438084,0.0236930679\C,-0.0422698672,0.0000109464,1.2059051017\C,1.1936824153,0.0000166301,2.0193028861\C,1.0991696752,0.0002166731,3.4091480598\C,2.2481144597,0.0002261048,4.19532875\C,3.5079416622,0.0000333153,3.5861162711\C,3.6002516913,-0.0001686548,2.1809370484\C,2.4562121743,-0.0001771707,1.4044539644\H,0.1164197789,0.000365307,3.8716640555\H,2.15066677,0.0003834815,5.2743109842\H,4.5788545528,-0.0003181899,1.7093027823\H,2.5201388821,-0.000332333,0.3205659221\S,5.0365799064,0.0000227566,4.4647437428\C,4.5080654279,0.0003069885,6.1931955015\H,5.4267407958,0.0003089471,6.7813755601\H,3.9350450386,0.8977140626,6.4345043511\H,3.9348902245,-0.8969345427,6.4347521305\\Version=ES64L-G09RevD.01\State=2-A'\HF=-782.238338\S2=0.753875\S2-1=0.\S2A=0.75001\RMSD=3.390e-09\RMSF=2.615e-05\Dipole=0.8370127,0.000142,1.5516457\Quadrupole=-3.7364408,-0.5107225,4.2471633,-0.0005044,-5.6687732,0.0011459\PG=CS [SG(C8H5O1S1),X(H2)]\\@

T cation

1\1\GINC-R77\FOpt\RM062X\6-31+G(d,p)\C8H7O1S1(1+)\ROOT\23-Mar-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\T_cat.2.freq\\1,1\O,-0.1413568393,-4.3463249344,0.\C,-0.1496995977,-3.2131390252,0.\C,-0.1604963448,-1.8375777793,0.\C,1.0750869327,-1.1336579658,0.\C,1.0593666787,0.2380987316,0.\C,-0.1702597808,0.945354577,0.\C,-1.396807705,0.2219712569,0.\C,-1.4073876735,-1.1449019163,0.\H,2.0158419703,-1.6741800292,0.\H,2.0021626626,0.7703495955,0.\H,-2.3362614118,0.7654625325,0.\H,-2.3431614891,-1.6933118612,0.\S,-0.3053815513,2.6582309536,0.\C,1.4072782177,3.2416671029,0.\H,1.3344023316,4.3298998753,0.\H,1.9316583002,2.9240554428,0.9024695661\H,1.9316583002,2.9240554428,-0.9024695661\\Version=ES64L-G09RevD.01\State=1-A'\HF=-782.0116256\RMSD=3.950e-09\RMSF=7.825e-06\Dipole=0.4442322,-0.8465018,0.\Quadrupole=-0.8350562,14.4296484,-13.5945922,5.5045631,0.,0.\PG=CS [SG(C8H5O1S1),X(H2)]\\@

T rad $AlCl_3$

1\1\GINC-R37\FOpt\UM062X\6-31+G(d,p)\C8H7Al1Cl3O1S1(2)\ROOT\15-Feb-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\T_rad_AlCl3.2.CS.freq\\0,2\O,0.,0.3319916398,1.1565375781\C,0.,-0.455567554,0.2313653942\C,0.,-0.2047686514,-1.1791814409\C,0.,-1.2908042855,-2.0646504151\C,0.,-1.0728681213,-3.4332234616\C,0.,0.2401870714,-3.9311635641\C,0.,1.3320679844,-3.0336719804\C,0.,1.1178520213,-1.6734806044\H,0.,-2.3007116775,-1.6657201535\H,0.,-1.9224401435,-4.1044567746\H,0.,2.3448383604,-3.4250448937\H,0.,1.9503900265,-0.976994099\Al,0.,0.0182732506,3.0593552265\Cl,-1.7952842836,0.9631228045,3.6309719869\Cl,1.7952842836,0.9631228045,3.6309719869\Cl,0.,-2.0980722094,3.1376050619\S,0.,0.6471110889,-5.632836964\C,0.,-0.9679455839,-6.4453460387\H,0.,-0.7547232668,-7.5149523849\H,0.898596845,-1.5365227792,-6.19935223\H,-0.898596845,-1.5365227792,-6.19935223\\Version=ES64L-G09RevD.01\State=2-A'\HF=-2405.3840276\S2=0.755658\S2-1=0.\S2A=0.750019\RMSD=4.870e-09\RMSF=1.743e-05\Dipole=0.,-0.5232694,-5.1089701\Quadrupole=-6.1216116,2.1131376,4.0084739,0.,0.,6.3136786\PG=CS [SG(C8H5Al1Cl1O1S1),X(H2Cl2)]\\@

T cation $AlCl_3$

1\1\GINC-R37\FOpt\UM062X\6-31+G(d,p)\C8H7Al1Cl3O1S1(2)\ROOT\15-Feb-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\T_rad_AlCl3.2.CS.freq\\0,2\O,0.,0.3319916398,1.1565375781\C,0.,-0.455567554,0.2313653942\C,0.,-0.2047686514,-1.1791814409\C,0.,-1.2908042855,-2.0646504151\C,0.,-1.0728681213,-3.4332234616\C,0.,0.2401870714,-3.9311635641\C,0.,1.3320679844,-3.0336719804\C,0.,1.1178520213,-1.6734806044\H,0.,-2.3007116775,-1.6657201535\H,0.,-1.9224401435,-

4.1044567746\H,0.,2.3448383604,-3.4250448937\H,0.,1.9503900265,-0.976994099\Al,0.,0.0182732506,3.0593552265\Cl,-1.7952842836,0.9631228045,3.6309719869\Cl,1.7952842836,0.9631228045,3.6309719869\Cl,0.,-2.0980722094,3.1376050619\S,0.,0.6471110889,-5.632836964\C,0.,-0.9679455839,-6.4453460387\H,0.,-0.7547232668,-7.5149523849\H,0.898596845,-1.5365227792,-6.19935223\H,-0.898596845,-1.5365227792,-6.19935223\\Version=ES64L-G09RevD.01\State=2-A'\HF=-2405.3840276\S2=0.755658\S2-1=0.\S2A=0.750019\RMSD=4.870e-09\RMSF=1.743e-05\Dipole=0.,-0.5232694,-5.1089701\Quadrupole=-6.1216116,2.1131376,4.0084739,0.,0.,6.3136786\PG=CS [SG(C8H5Al1Cl1O1S1),X(H2Cl2)]\\@

T rad-H

1\1\GINC-R1614\FOpt\RM062X\6-31+G(d,p)\C8H8O1S1\ROOT\15-Feb-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\T_radH.2.freq\\0,1\O,-0.059858593,-0.00020924,-0.0145241565\C,-0.0402670299,-0.0000436572,1.1961408497\C,1.1930634739,-0.0000260785,2.0116520285\C,1.106113901,0.0001725183,3.4020754138\C,2.2555522682,0.0001926098,4.1889852308\C,3.5134443842,0.0000113582,3.5775713531\C,3.6007248452,-0.0001893657,2.1719203189\C,2.4542199739,-0.0002077162,1.3992621653\H,0.1287034278,0.0003137262,3.8798482175\H,2.1595965443,0.0003489431,5.2681623828\H,4.5781272738,-0.000330055,1.6979006749\H,2.5090415631,-0.0003616041,0.3148519793\S,5.0456634727,0.0000141852,4.4529654345\C,4.5214899641,0.0002932624,6.1825596874\H,5.4409545807,0.0003034782,6.7695992883\H,3.9487489254,0.8975573984,6.4253254114\H,3.9486107461,-0.8968156073,6.425573064\H,-0.9870229896,0.0001093518,1.7765232941\\Version=ES64L-G09RevD.01\State=1-A'\HF=-782.8899869\RMSD=3.224e-09\RMSF=1.243e-04\Dipole=0.3286852,0.0002206,1.7817906\Quadrupole=0.5859045,-1.0564356,0.4705311,-0.0009388,-5.8858685,0.000664\PG=CS [SG(C8H6O1S1),X(H2)]\\@

T rad-H $AlCl_3$

1\1\GINC-R39\FOpt\RM062X\6-31+G(d,p)\C8H8Al1Cl3O1S1\ROOT\15-Feb-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\T_radH_AlCl3.2.CS.freq\\0,1\O,0.,-0.1719484453,-1.0816570934\C,0.,0.7763094731,-0.2730905011\C,0.,0.5718065669,1.1478862211\C,0.,1.6890672438,2.0031456459\C,0.,1.5144978016,3.3719488406\C,0.,0.215308606,3.9187192769\C,0.,-0.9024388995,3.0623525058\C,0.,-0.7240126293,1.6915284595\H,0.,2.6913948633,1.5829820394\H,0.,2.374947474,4.0336257517\H,0.,-1.9078386004,3.4648078776\H,0.,-1.5778938315,1.0211407369\H,0.,1.8028108941,-0.6648142461\Al,0.,-0.1454965879,-2.9649690033\Cl,-1.7972889351,-1.1420707923,-3.4464029985\Cl,1.7972889351,-1.1420707923,-3.4464029985\Cl,0.,1.9507089874,-3.3566230759\S,0.,0.1132079387,5.6658341801\C,0.,-1.6675900181,5.9800494934\H,0.,-1.7698665987,7.0659383035\H,-0.8985748728,-2.1416463269,5.5814702921\H,0.8985748728,-2.1416463269,5.5814702921\\Version=ES64L-G09RevD.01\State=1-A'\HF=-2406.055013\RMSD=5.802e-09\RMSF=3.001e-05\Dipole=0.,0.1464287,4.900562\Quadrupole=-5.367638,6.4152356,-1.0475976,0.,0.,-8.1971653\PG=CS [SG(C8H6Al1Cl1O1S1),X(H2Cl2)]\\@

D rad

1\1\GINC-R2763\FOpt\UM062X\6-31+G(d,p)\C9H11O2(2)\ROOT\09-Jan-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\BenzylOCH32_radical.freq\\0,2\C,0.1343046617,-0.9601586903,0.4278843879\O,-0.2059009578,-0.2047412526,1.4988133435\O,0.7038472387,-0.3237002648,-0.620873634\C,-0.1844964239,-2.3311859132,0.3530545289\C,-0.9102692694,-2.9608360707,1.398982846\C,-1.2180621032,-4.3088696128,1.321500091\C,-0.8225538579,-5.0722865376,0.2168845987\C,-0.1068636224,-4.4605276272,-0.819028841\C,0.2124478448,-3.1141206809,-0.7633817142\C,-1.2399836646,0.7496627103,1.2324362883\C,1.7657550748,0.5697029163,-0.2851607665\H,-1.208189148,-2.3717124283,2.2597783668\H,-1.7716524415,-4.7762679381,2.13042404889\H,-1.0675097845,-6.1277606308,0.1645632118\H,0.20276383,-5.045892557,-1.6797336945\H,0.7630759148,-2.6393622141,-1.5679343128\H,-1.3819227794,1.3168954576,2.1519551256\H,-2.1656012523,0.2300679424,0.9627688554\H,-0.9494909831,1.4219922307,0.4187638088\H,2.1352453318,0.9680617331,-1.2292682391\H,2.5630335082,0.0277697753,0.2339807923\H,1.4111528832,1.3856096529,0.3509244684\\Version=ES64L-G09RevD.01\State=2-A\HF=-499.7679216\S2=0.773156\S2-1=0.\S2A=0.75033\RMSD=5.958e-09\RMSF=1.750e-06\Dipole=0.0449366,0.8953226,0.0129258\Quadrupole=-1.0358011,4.465615,-3.4298138,1.2553024,-3.6527728,0.7543767\PG=C01 [X(C9H11O2)]\\@

D cation

1\1\GINC-R51\FOpt\RM062X\6-31+G(d,p)\C9H11O2(1+)\ROOT\23-Mar-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=2147483648\\D_cat.C2V.freq\\1,1\C,0.,0.,0.9324821009\O,-0.2363621205,1.1130857787,1.5429299822\O,0.2363621205,-1.1130857787,1.5429299822\C,0.,0.,-0.509469609\C,-0.0551221659,1.223680634,-1.2037619711\C,-0.0566645651,1.2154208446,-2.5892192584\C,0.,0.,-3.2777348646\C,0.0566645651,-1.2154208446,-2.5892192584\C,0.0551221659,-1.223680634,-1.2037619711\C,0.2671102471,1.4409280765,2.8687422237\C,-0.2671102471,-1.4409280765,2.8687422237\H,-0.0942883036,2.1583711987,-0.655709874\H,-0.0984510158,2.1501362308,-3.1366161211\H,0.,0.,-4.3631247046\H,0.0984510158,-2.1501362308,-3.1366161211\H,0.0942883036,-2.1583711987,-0.655709874\H,-0.4866069515,1.2011541467,3.6164345736\H,0.4356955437,2.5144729754,2.8346982457\H,1.2040213101,0.913281673,3.0474807378\H,-0.4356955437,-2.5144729754,2.8346982457\H,-1.2040213101,-0.913281673,3.0474807378\H,0.4866069515,-1.2011541467,3.6164345736\\Version=ES64L-G09RevD.01\State=1-A\HF=-499.5629921\RMSD=8.777e-09\RMSF=6.818e-06\Dipole=0.,0.,1.7075529\Quadrupole=-15.9742009,-3.1488135,19.1230144,1.5323711,0.,0.\PG=C02 [C2(C1C1C1H1),X(C6H10O2)]\\@

D rad $AlCl_3$

1\1\GINC-R123\FOpt\UM062X\6-31+G(d,p)\C9H11Al1Cl3O2(2)\ROOT\13-Jan-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653184\\BenzylOCH32_radical_AlCl3.test.freq\\0,2\C,0.9386186907,-0.2783283943,0.7445694845\O,1.8772372976,0.7698636568,0.8281448229\O,0.8633650608,-1.0431982203,1.8348807019\C,-0.174753764,-0.1165034916,-0.1313091796\C,-0.1896131474,0.9107453909,-1.1001473259\C,-1.267964289,1.0292297951,-1.9652737706\C,-2.3402349106,0.137288606,-1.8894337337\C,-2.3279803656,-0.8830620276,-0.9344485764\C,-1.259585372,-1.0171647066,-0.060434522\C,1.5313917868,1.8219478684,1.783271839\C,2.0970534512,-1.6333547639,2.2780638744\H,0.6464351956,1.6002953384,-1.1772164861\H,-1.2696852714,1.819873215,-2.7084719419\H,-3.1782654524,0.2346288604,-2.5714841647\H,-3.159218153,-1.5781441773,-0.8732058009\H,-1.243744291,-1.8063561122,0.683088691\H,2.2768310566,2.6081918694,1.6714431277\H,1.5581978567,1.3945069203,2.7858771467\H,0.5365057811,2.1859887521,1.5238028733\H,1.8343657957,-2.2657428336,3.1238909204\H,2.80480473,-0.8608071119,2.5932388669\H,2.5327363544,-2.2279888758,1.4707200243\Al,3.5551557836,0.8193571441,-0.082352888\Cl,3.3846215026,2.6295704523,-1.1654125792\Cl,4.89558273,0.9169671676,1.5583261726\Cl,3.542171943,-0.9774043214,-1.1813275766\\Version=ES64L-G09RevD.01\State=2-A\HF=-2122.9294557\S2=0.769699\S2-1=0.\S2A=0.750229\RMSD=4.908e-09\RMSF=1.903e-06\Dipole=-1.9567998,-0.2292406,1.184903\Quadrupole=-3.7643001,0.9573714,2.8069287,-1.6145091,3.261334,-1.6926957\PG=C01 [X(C9H11Al1Cl3O2)]\\@

D cation $AlCl_3$

1\1\GINC-R197\FOpt\RM062X\6-31+G(d,p)\C9H11Al1Cl3O2(1+)\ROOT\24-Mar-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653184\\D_rad_AlCl3.freq\\1,1\C,0.9420556609,-0.3088146248,0.7649010182\O,1.8624088553,0.6624091503,0.9513397997\O,1.1167281132,-1.4012435351,1.3826662653\C,-0.1892505436,-0.1147855425,-0.0803217652\C,-0.1789911163,0.9339746433,-1.026465039\C,-1.2606960615,1.0812356973,-1.8771200949\C,-2.3441704325,0.2010893275,-1.7831834018\C,-2.3525945799,-0.8437614976,-0.8507933319\C,-1.2741525997,-1.0162334287,-0.0027063271\C,1.414282086,1.9165683848,1.6172982226\C,2.254204405,-1.6526429444,2.2703416002\H,0.684715609,1.5864881975,-1.1235626256\H,-1.2605367123,1.8691055586,-2.6215844733\H,-3.1910981975,0.3260326741,-2.4506409724\H,-3.1993947644,-1.5182822847,-0.7966710632\H,-1.2592299571,-1.8217445904,0.7237496183\H,2.321862577,2.3189962308,2.0655980369\H,0.6832350594,1.6459753128,2.3780001637\H,1.0051611158,2.5852147266,0.8635685486\H,1.9237143829,-2.4726637865,2.901153461\H,2.4831456216,-0.7562636448,2.8448294286\H,3.0942518158,-1.9477789714,1.6403553973\Al,3.6705575685,0.7292344238,-0.1052131514\Cl,3.2935689221,2.5273891543,-1.1070463758\Cl,4.921815599,0.741725353,1.5668448143\Cl,3.3024375735,-1.0808239837,-1.1065377531\\Version=ES64L-G09RevD.01\State=1-A\HF=-2122.6859989\RMSD=3.944e-09\RMSF=6.074e-06\Dipole=-3.40381,-0.533023,1.436185\Quadrupole=7.6357634,-6.2059,-1.4298633,1.0474604,7.7654565,-5.0772865\PG=C01 [X(C9H11Al1Cl3O2)]\\@

D rad-H

1\1\GINC-R2085\FOpt\RM062X\6-31+G(d,p)\C9H12O2\ROOT\08-Jan-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\BenzylOCH32_radicalH.freq\\0,1\C,-0.7080328315,-0.7437452736,0.027686869\O,-0.9689579064,-0.2049585154,1.2904779185\O,0.3857581639,-0.1188490434,-0.5998908275\C,-0.5184232892,-2.2433596052,0.1648688796\C,-0.7886755724,-2.9178594375,1.3542253286\C,-0.6177316885,-4.3012678921,1.4257540146\C,-0.1790104829,-5.0136964133,0.3124845514\C,0.0916118096,-4.3391009527,-0.8790939093\C,-0.0781486444,-2.9597182643,-0.9515612771\C,-1.3160834748,1.1663467163,1.2487793621\C,1.6092193782,-0.2292612784,0.1120566207\H,-1.1273941002,-2.354899332,2.2166357723\H,-0.8274385317,-4.8217233842,2.3552054215\H,-0.0472214463,-6.0896641635,0.3708696104\H,0.4356531103,-4.888379843,-1.749988834\H,0.1410370792,-2.4242091492,-1.8716748424\H,-1.559880368,1.4604364171,2.2698842412\H,-2.1906347506,1.3254533763,0.6039364446\H,-0.4859147666,1.7753012126,0.8751139392\H,2.348232031,0.3284236376,-0.4637081571\H,1.9258481896,-1.2750571959,0.1993019143\H,1.5216023593,0.2013920037,1.1156285803\H,-1.5496442675,-0.52799362,-0.6485816209\\Version=ES64L-G09RevD.01\State=1-A\HF=-500.4159255\RMSD=6.135e-09\RMSF=6.085e-06\Dipole=0.0583996,0.1256399,0.1364689\Quadrupole=-1.7088187,3.1991295,-1.4903108,-1.4976818,-0.8697215,1.7768807\PG=C01 [X(C9H12O2)]\\@

D rad-H $AlCl_3$

1\1\GINC-R362\FOpt\RM062X\6-31+G(d,p)\C9H12Al1Cl3O2\ROOT\18-Jan-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653184\\BenzylOCH32_radicalH_AlCl3.freq\\0,1\C,0.629673362,-0.9542820035,0.2702479178\O,-0.3815474623,-0.2727372673,-0.569276562\O,0.6818775402,-2.2764418661,-0.0707571861\C,1.9620172319,-0.2776424818,0.0735391256\C,2.0249187343,1.1155656522,0.1672823838\C,3.2457378985,1.7650728929,0.0156513079\C,4.4045876209,1.0256956918,-0.2260347219\C,4.3390861825,-0.3626025188,-0.3161051929\C,3.1172069295,-1.0190434209,-0.1663241173\C,-0.1697834358,-0.4164201934,-1.9976644181\C,-0.4777524737,-3.0157802346,0.3128376297\H,1.118630651,1.6906111999,0.3447969132\H,3.2921958081,2.8468213159,0.085447067\H,5.3566869046,1.5332707348,-0.3436821662\H,5.2391920567,-0.9388407402,-0.5043499403\H,3.0536712911,-2.0993532951,-0.2347946552\H,-0.7628812658,0.3576823733,-2.4838662975\H,-0.4960865187,-1.4094951196,-2.3073795918\H,0.890003725,-0.2640601935,-2.2029555387\H,-0.2699237327,-4.0579998025,0.0761523182\H,-1.3587248589,-2.6779443122,-0.2448573223\H,-0.6627561091,-2.9046899419,1.3868367791\Al,-2.0298213425,0.4762937029,-0.0123505289\Cl,-1.8526252051,2.4762655507,-0.6793350698\Cl,-3.4297573264,-0.7058194591,-1.0795135481\Cl,-2.0238297388,0.1996876172,2.087253973\H,0.2370335334,-0.8013638812,1.2813314417\\Version=ES64L-G09RevD.01\State=1-A\HF=-2123.5841321\RMSD=3.352e-09\RMSF=4.775e-06\Dipole=2.2285232,-1.1306041,-0.5285364\Quadrupole=-1.8687225,3.4691826,-1.60046,3.8114449,-1.3260762,-0.2039423\PG=C01 [X(C9H12Al1Cl3O2)]\\@

M rad

1\1\GINC-R99\FOpt\UM062X\6-31+G(d,p)\C7H14N1O1(2)\ROOT\16-Feb-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\M_rad.freq\\0,2\C,0.0989343365,-1.2836989388,2.4704186933\C,-0.1545180055,0.,1.7351056527\C,0.0989343365,1.2836989388,2.4704186933\N,0.1054157035,0.,0.3525352348\C,-0.2840565265,-1.2005809574,-0.3847642822\C,-0.2840565265,1.2005809574,-0.3847642822\C,0.266096371,-1.1578949812,-1.8022250723\O,-0.1610378868,0.,-2.4897391045\C,0.266096371,1.1578949812,-1.8022250723\H,-0.0600870935,-1.1321544709,3.5398364265\H,1.1354900288,-1.6394198892,2.3364526063\H,-0.5657282312,-2.0959527357,2.1589839149\H,1.1354900288,1.6394198892,2.3364526063\H,-0.0600870935,1.1321544709,3.5398364265\H,-0.5657282312,2.0959527357,2.1589839149\H,-1.3849308965,-1.2900390141,-0.4182956725\H,0.1180469171,-2.0837849493,0.1151807308\H,0.1180469171,2.0837849493,0.1151807308\H,-1.3849308965,1.2900390141,-0.4182956725\H,-0.0944877541,-2.0162215587,-2.3738673018\H,1.3669379428,-1.1852853562,-1.7699009346\H,1.3669379428,1.1852853562,-1.7699009346\H,-0.0944877541,2.0162215587,-2.3738673018\\Version=ES64L-G09RevD.01\State=2-A'\HF=-404.9143146\S2=0.753945\S2-1=0.\S2A=0.750012\RMSD=5.635e-09\RMSF=5.420e-06\Dipole=0.2290699,0.,0.3513634\Quadrupole=-1.3089935,4.5556797,-3.2466861,0.,-0.84099,0.\PG=CS [SG(C1N1O1),X(C6H14)]\\@

M cation

1\1\GINC-R85\Freq\RM062X\6-31+G(d,p)\C7H14N1O1(1+)\ROOT\19-Mar-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) SCF=tight Freq=(noraman) maxdisk=268435456\\M_cat.freq\\1,1\C,-0.1990842409,-1.2775347443,-2.3657910273\C,0.0579478926,0.0072362354,-1.6357614347\C,-0.0242956104,1.2832648745,-2.4167930414\N,0.3459785717,0.008407483,-0.3718675358\C,0.5077165423,-1.2135899925,0.450148073\C,0.4936778994,1.2282448435,0.4565126982\C,-0.4958352904,-1.1751482441,1.6041422596\O,-0.3048841009,-0.0142792325,2.3737227755\C,-0.5074898663,1.1499748429,1.6139497884\H,-0.62673123,-1.0668497347,-3.344573862\H,-0.8827613774,-1.9312872923,-1.8210282919\H,0.7440329257,-1.8157170732,-2.5195001029\H,0.0857359539,1.0665633093,-3.4787383962\H,0.7382014538,2.0065382078,-2.126644244\H,-1.0115646787,1.7402494587,-2.2745704625\H,1.527086529,-1.1864450657,0.8473203451\H,0.3895890352,-2.1042057668,-0.1616359555\H,0.3140872581,2.1182592606,-0.1411811785\H,1.5177703333,1.2407864459,0.8409202976\H,-0.3313964439,-2.0323259489,2.2585948631\H,-1.5240977895,-1.2169840081,1.2125379891\H,-1.534935857,1.1813676113,1.2194673318\H,-0.3575245206,2.0034745303,2.2767991062\\Version=ES64L-G09RevD.01\State=1-A\HF=-404.7356465\RMSD=2.867e-09\RMSF=3.377e-07\ZeroPoint=0.210797\Thermal=0.2202671\Dipole=0.1563615,0.0098714,-1.7130999\
PG=C01 [X(C7H14N1O1)]\\@

M rad (O) $AlCl_3$

1\1\GINC-R2542\FOpt\UM062X\6-31+G(d,p)\C7H14Al1Cl3N1O1(2)\ROOT\18-Feb-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653184\\M_rad_AlCl3.Ob.CS.freq\\0,2\C,-0.28013,-1.19693,-2.02289\C,0.33267,-1.19433,-0.63983\O,-0.0958,0.,0.07283\C,0.33267,1.19433,-0.63983\C,-0.28013,1.19693,-2.02289\N,0.10153,0.,-2.7653\H,-1.37794,-1.27918,-1.94047\H,0.09187,-2.08515,-2.53624\H,1.42742,-1.17753,-0.67724\H,-0.01488,-2.0419,-0.04866\H,1.42742,1.17753,-0.67724\H,-0.01488,2.0419,-0.04866\H,0.09187,2.08515,-2.53624\H,-1.37794,1.27918,-1.94047\C,-0.20779,0.,-4.14401\C,0.01558,-1.28636,-4.8825\C,0.01558,1.28636,-4.8825\H,1.05144,-1.65022,-4.77401\H,-0.16803,-1.13407,-5.94734\H,-0.65046,-2.09185,-4.5563\H,1.05144,1.65022,-4.77401\H,-0.65046,2.09185,-4.5563\H,-0.16803,1.13407,-5.94734\Al,-0.02782,0.,1.97884\Cl,-1.022,-1.79633,2.47868\Cl,-1.022,1.79633,2.47868\Cl,2.0721,0.,2.27725\\Version=ES64L-G09RevD.01\State=2-A'\HF=-2028.0806454\S2=0.754046\S2-1=0.\S2A=0.750013\RMSD=1.850e-09\RMSF=5.842e-06\Dipole=0.1537277,0.,-2.9019471\Quadrupole=-2.6297477,4.7717161,-2.1419684,0.,-0.1856608,0.\PG=CS [SG(C1Al1Cl1N1O1),X(C6H14Cl2)]\\@

M cation (O) $AlCl_3$

1\1\GINC-R78\FOpt\RM062X\6-31+G(d,p)\C7H14Al1Cl3N1O1(1+)\ROOT\24-Mar-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653184\\M_rad_AlCl3.Ob.2.freq\\1,1\N,-0.224638194,-0.296675774,0.075408516\C,-0.0838072435,-0.1665130103,1.5450370604\C,1.379934744,0.0369409342,1.9138952956\C,0.6532436866,-1.3587116256,-0.470477302\C,2.0944072424,-1.1186598333,-0.0402261648\O,2.1759808296,-1.0450585562,1.3955019843\C,-1.0653704181,0.3893105214,-0.6376083514\C,-1.9559313808,1.4084550979,0.0083119026\C,-1.1748745267,0.1587750312,-2.1154042219\H,0.2936291411,-2.3119033504,-0.0680221319\H,0.5973631956,-1.3779844218,-1.5562241531\H,2.4931074683,-0.1807941657,-0.4409849305\H,2.7295705468,-1.9486676721,-0.3532855771\H,1.7825911042,0.9683521785,1.5022009379\H,1.5043207225,0.0331258421,2.9978122981\H,-0.6690493172,0.6740457706,1.9102362278\H,-0.4590039584,-1.0951958538,1.9884458446\H,-0.2255897846,0.3705703747,-2.6177585644\H,-1.9373060399,0.8057006331,-2.5427338581\H,-1.4463273355,-0.8808558797,-2.3259614818\H,-1.366436335,2.2074801177,0.4696899622\H,-2.5726853098,0.9480906662,0.7868154825\H,-2.6147076677,1.8567755443,-0.7315963022\Al,2.5735318421,-2.6451041132,2.4871799691\Cl,4.0888563717,-3.5101301225,1.3285210475\Cl,2.9927044859,-1.7365315866,4.3272124961\Cl,0.6633500168,-3.5760507524,2.3395113347\\Version=ES64L-G09RevD.01\State=1-A\HF=-2027.8802254\RMSD=3.765e-09\RMSF=1.449e-05\Dipole=-3.7681596,4.1964163,-3.8592654\Quadrupole=0.5072633,-2.1842851,1.6770218,-13.3810048,10.5119424,-7.5087047\PG=C01 [X(C7H14Al1Cl3N1O1)]\\@

M rad-H

1\1\GINC-R64\FOpt\RM062X\6-31+G(d,p)\C7H15N1O1\ROOT\16-Feb-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=268435456\\M_radH.freq\\0,1\C,0.1598710329,-1.2464775202,2.4735789861\C,-0.3179141664,0.,1.7258375803\C,0.1598710329,1.2464775202,2.4735789861\N,0.1710764559,0.,0.3374074766\C,-0.2605045801,-1.1878018806,-0.3984726962\C,-0.

2605045801,1.1878018806,-0.3984726962\C,0.2617431417,-1.1563897975,-1.8267382735\O,-0.1712828433,0.,-2.5129254016\C,0.2617431417,1.1563897975,-1.8267382735\H,-0.0850314003,-1.1554985356,3.534988108\H,1.2465757834,-1.3438369642,2.375414577\H,-0.3078772703,-2.1645933065,2.112566101\H,1.2465757834,1.3438369642,2.375414577\H,-0.0850314003,1.1554985356,3.534988108\H,-0.3078772703,2.1645933065,2.112566101\H,-1.3661481687,-1.262945199,-0.4173821549\H,0.1341292589,-2.0842346169,0.084954026\H,0.1341292589,2.0842346169,0.084954026\H,-1.3661481687,1.262945199,-0.4173821549\H,-0.1127736825,-2.015909901,-2.387678156\H,1.3627309197,-1.1893894765,-1.8124278699\H,1.3627309197,1.1893894765,-1.8124278699\H,-0.1127736825,2.015909901,-2.387678156\H,-1.4277795156,0.,1.7212150492\\Version=ES64L-G09RevD.01\State=1-A'\HF=-405.5677434\RMSD=7.028e-09\RMSF=6.383e-06\Dipole=0.0144567,0.,0.6047931\Quadrupole=-0.8717371,3.9559233,-3.0841862,0.,-1.6196396,0.\PG=CS [SG(C1H1N1O1),X(C6H14)]\\@

M rad-H (O) $AlCl_3$

1\1\GINC-R43\FOpt\RM062X\6-31+G(d,p)\C7H15Al1Cl3N1O1\ROOT\23-Feb-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653184\\M_radH_AlCl3.Ob.3.freq\\0,1\C,-1.9092194331,1.3572655168,0.049300293\C,-0.4663331235,1.2744204874,0.5064370258\O,0.1884045786,0.1369591588,-0.1276846661\C,-0.5144424571,-1.1065720069,0.1601890519\C,-1.9519045184,-0.9977906694,-0.3057379801\N,-2.6007944997,0.1165402416,0.3755572168\H,-1.9275122946,1.5905926038,-1.0284147456\H,-2.3847760998,2.1842825346,0.5874985856\H,-0.3973800875,1.1046255683,1.5849195679\H,0.1137450847,2.1543896297,0.2266578329\H,-0.4547538807,-1.2489223455,1.2432128715\H,0.0364988791,-1.8922964773,-0.3562981269\H,-2.4571314049,-1.9337461195,-0.0488979021\H,-1.9613169931,-0.8891873303,-1.4037731895\C,-4.0576537,0.1955940181,0.1634904018\C,-4.7689292129,-0.9219722465,0.9227813855\C,-4.4840967208,0.219529914,-1.3100950001\H,-4.5830634485,-1.9015745954,0.470257991\H,-5.8500545189,-0.7585247481,0.9009654569\H,-4.4377274931,-0.948809046,1.963737628\H,-4.3136066252,-0.7511180656,-1.7874371677\H,-3.9454073715,0.9796359474,-1.8839657804\H,-5.5528490891,0.438900869,-1.3849182367\H,-4.354938025,1.1467155261,0.6233276165\Al,1.2919857483,0.3631544244,-1.6592204503\Cl,-0.1076497558,0.7686064123,-3.2052880207\Cl,2.2660618139,-1.5072074867,-1.8181135837\Cl,2.4977046488,2.0121882847,-1.112838075\\Version=ES64L-G09RevD.01\State=1-A\HF=-2028.7363325\RMSD=5.891e-09\RMSF=3.524e-06\Dipole=-2.3526969,-0.2367625,1.7320277\Quadrupole=-2.4259349,2.7994475,-0.3735127,-0.6486813,1.5120907,0.7324342\PG=C01 [X(C7H15Al1Cl3N1O1)]\\@

M rad (N) $AlCl_3$

1\1\GINC-R1475\FOpt\UM062X\6-31+G(d,p)\C7H14Al1Cl3N1O1(2)\ROOT\17-Feb-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653184\\N_rad_AlCl3.freq\\0,2\C,-2.0988462328,0.5753446942,0.6175709982\C,-0.5945637435,0.7374714739,0.7786822434\O,0.0940503992,0.1367080309,-0.2960009809\C,-0.1673130235,-1.2495362588,-0.2878885974\C,-1.6475030489,-1.5239535221,-0.5089940132\N,-2.525372079,-0.8711328034,0.5324810267\H,-2.407386155,1.0492002087,-0.3220317226\H,-2.6183757203,1.0494334272,1.4504228171\H,-0.2505036378,0.3183555073,1.7331294374\H,-0.3587180584,1.8037902834,0.7637073007\H,0.1831044779,-1.6974558956,0.6510206471\H,0.3931184916,-1.6933780981,-1.1136063738\H,-1.8340910624,-2.5979717658,-0.5067817788\H,-1.9446052416,-1.1041314498,-1.4775266007\C,-3.9291492172,-0.9344563564,0.0881206917\C,-4.8770393276,0.0670807376,0.6674548375\C,-4.3883534018,-2.2055616377,-0.5526604119\H,-4.7528151522,0.1903428921,1.7519964811\H,-5.9009033287,-0.2709420307,0.5025444149\H,-4.7730620951,1.0587448282,0.2100451416\H,-4.0454111835,-3.0996473489,-0.0142936359\H,-4.0511293117,-2.2985663287,-1.5924034378\H,-5.4787353254,-2.2342160127,-0.5515169165\Al,-2.509369917,-1.8486938828,2.3606246722\Cl,-1.8855334075,-0.3890649456,3.7768132561\Cl,-1.2121518601,-3.5143926519,2.1000670758\Cl,-4.4907618377,-2.5021010947,2.782683428\\Version=ES64L-G09RevD.01\State=2-A\HF=-2028.0786879\S2=0.755058\S2-1=0.\S2A=0.750021\RMSD=8.299e-09\RMSF=5.509e-06\Dipole=-0.4232896,1.1019751,-2.2234301\Quadrupole=0.2454649,1.1737416,-1.4192065,-2.6439279,3.5812471,3.4662211\PG=C01 [X(C7H14Al1Cl3N1O1)]\\@

M cation (N) AlCl

1\1\GINC-R37\FOpt\RM062X\6-31+G(d,p)\C7H14Al1Cl3N1O1(1+)\ROOT\10-Jun-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=671088640\\M_rad_AlCl3.freq\\1,1\C,-2.0482333203,0.7961752646,0.3041122481\C,-0.5822566428,0.7700332223,0.7281791658\O,0.2059976203,0.1339153473,-0.2455942147\C,-0.1540043456,-1.2209444443,-0.3403473554\C,-1.5832751642,-1.3655339786,-0.8559988268\N,-2.5385904502,-0.5643741248,-0.0444542656\H,-2.1636128442,1.4049138644,-0.6003020632\H,-2.66226598,1.2091966871,1.1022388906\H,-0.4750890989,0.2672773956,1.6995819773\H,-0.2298979223,1.7983535869,0.8237295879\H,-0.0482800932,-1.7169746028,0.6346613773\H,0.5220026479,-1.6972671667,-1.0522902785\H,-1.8834116188,-2.4116235539,-0.8408902684\H,-1.6508833685,-0.97895585,-1.8796330621\C,-3.7733875178,-0.9282630776,0.1388502004\C,-4.7469796237,-0.0041185445,0.8094825375\C,-4.2658166403,-2.242534928,-0.3921026854\H,-4.415491679,0.284126873,1.8127731842\H,-5.7206166014,-0.4811142646,0.8961167674\H,-4.8517687885,0.9141454518,0.2200074127\H,-3.6912660094,-3.0867803233,0.0037692376\H,-4.1689043685,-2.2603736017,-1.4838648837\H,-5.310875351,-2.3877361853,-0.127966728\Al,-2.942780169,-2.3702184166,3.1581912194\Cl,-2.2947798317,-0.5084112602,3.8060733672\Cl,-1.6286639577,-3.6122882652,2.1401864921\Cl,-4.9682888812,-2.7893551051,3.1291509664\\Version=ES64L-G09RevD.01\State=1-A\HF=-2027.8460616\RMSD=3.883e-09\RMSF=1.331e-05\Dipole=-0.9690429,0.7755644,-1.8333067\Quadrupole=-4.1676924,-0.7233202,4.8910126,-2.0894555,2.9760821,-2.9952875\PG=C01 [X(C7H14Al1Cl3N1O1)]\\@

M rad-H (N) $AlCl_3$

1\1\GINC-R1247\FOpt\RM062X\6-31+G(d,p)\C7H15Al1Cl3N1O1\ROOT\18-Feb-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653184\\M_radH_AlCl3.1.freq\\0,1\C,-1.5063562092,0.767078928,-1.2113246672\C,-2.54184188,-0.3576112378,-1.1826192828\O,-3.2980462733,-0.3141346903,0.0101890729\C,-2.4363288264,-0.4862243651,1.1150437948\C,-1.486936

7608,0.694852395,1.2248778076\N,-0.6199806192,0.8226387157,0.0056275846\H,-2.063163132,1.704647006,-1.2590292844\H,-0.8683529991,0.6882747798,-2.0984552161\H,-2.0848566796,-1.3429267222,-1.2987333685\H,-3.2355651509,-0.1943630767,-2.0105848979\H,-1.8841344085,-1.4352314691,1.0301359832\H,-3.0579984436,-0.5304243561,2.0115221828\H,-0.8473691052,0.5912504889,2.100957895\H,-2.088075053,1.6049936025,1.3189221699\C,0.1112141375,2.1719639752,0.0304737738\C,0.8993211529,2.3387090343,1.3305004526\C,-0.7775693507,3.4009667269,-0.1892703566\H,0.8139399575,2.1168127416,-0.8033382323\H,0.2449665343,2.6451834285,2.1525477717\H,1.6419349752,3.1258551134,1.1813779435\H,1.4401074088,1.4403184938,1.6353184173\H,-1.632713428,3.4406908987,0.4911158797\H,-1.1368011832,3.4983006617,-1.2144862698\H,-0.1629119683,4.2809345164,0.0175439362\Al,0.8359681054,-0.644532956,-0.0627311439\Cl,0.2630540907,-2.1984659463,-1.3964298873\Cl,1.0071894679,-1.3319518576,1.9474301065\Cl,2.603695641,0.2796951706,-0.8112321655\\Version=ES64L-G09RevD.01\State=1-A\HF=-2028.7358907\RMSD=7.994e-09\RMSF=7.624e-06\Dipole=-1.6031446,2.2963796,0.1345859\Quadrupole=-6.3182775,3.4574698,2.8608077,1.2180454,1.2189034,-0.19445\PG=C01 [X(C7H15Al1Cl3N1O1)]\\@

B rad-MMA TS

1\1\GINC-R517\Freq\UM062X\6-31+G(d,p)\C12H13O3(2)\ROOT\03-Jul-2014\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/6-31+G(d,p) Freq\\B_MMA_TS.freq\\0,2\C,0.0930210166,-0.1307647429,0.0676060053\C,0.1130935202,-0.1202924545,1.4646130052\C,1.3215402387,-0.0319410986,2.1542155848\C,2.5187088307,0.0443339524,1.446758682\C,2.4976197324,0.0357776715,0.0514440108\C,1.2841853236,-0.051616661,-0.6436710399\H,-0.8518619866,-0.1996485391,-0.4617546676\H,-0.8193895347,-0.1813271136,2.0170620541\H,1.3302494889,-0.0230960947,3.2390442483\H,3.4673079952,0.1139944747,1.969374815\C,3.7686211463,0.1169214616,-0.714298094\H,1.2964587378,-0.0556074022,-1.7292916138\O,3.9118994141,0.1713829758,-1.887864431\C,5.8135819582,0.0477260824,0.4740573738\C,6.7109533945,0.0177213906,-0.5426845238\H,5.5243658514,-0.8763651364,0.9681669253\H,5.5662745087,0.983010848,0.9647566831\C,7.1729871106,-1.2428138363,-1.2067580853\C,7.1933647316,1.2726488076,-1.1586268694\O,8.0019016747,1.316567269,-2.0628105463\O,6.6456216985,2.3840945553,-0.6217342633\C,7.0863109082,3.6108790432,-1.2002002776\H,8.262618312,-1.2616866128,-1.2961265982\H,6.7704235994,-1.303381346,-2.2245302211\H,6.8416393749,-2.1192221652,-0.6455475175\H,6.5556905894,4.3971673478,-0.6655852084\H,6.8444214485,3.636869045,-2.2648945309\H,8.1661564528,3.7229452418,-1.079597656\\Version=ES64L-G09RevD.01\State=2-A\HF=-690.4339911\S2=0.774295\S2-1=0.\S2A=0.750167\RMSD=2.629e-09\RMSF=6.830e-07\ZeroPoint=0.2235059\Thermal=0.2389367\Dipole=-1.7644349,-0.0216462,1.4257628\PG=C01 [X(C12H13O3)]\\@

B rad-MMA

1\1\GINC-R145\FOpt\UM062X\6-31+G(d,p)\C12H13O3(2)\ROOT\06-Mar-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=402653184\\B_MMA_rad.6.freq\\0,2\C,-3.7385713153,-0.7434955799,0.3757171796\C,-3.1819394087,-2.0222354816,0.2979372661\C,-1.8457453204,-2.1820914968,-0.0622762954\C,-1.0585829342,-1.0676941476,-0.3488721655\C,-1.6141179224,0.2143940353,-0.2702595873\C,-2.9576463013,0.3703189528,0.0938049045\H,-4.7797062794,-0.6194234481,0.6560074516\H,-3.7919736106,-2.8931078912,0.5177247324\H,-1.4120670566,-3.1749550462,-0.1234992932\H,-0.0181951538,-1.2101966419,-0.6265090194\C,-0.8208042635,1.449171477,-0.5623505491\H,-3.3658307772,1.3743992427,0.1482876794\O,-1.3186798744,2.5540513883,-0.4710343514\C,0.6614797796,1.3149422751,-0.9273308224\C,1.4733736215,1.1223541084,0.3134317551\H,0.9326769789,2.2641892484,-1.4034565897\H,0.8371675301,0.493194039,-1.6242753217\C,1.5157945809,2.1875760004,1.3551987164\C,2.2677476425,-0.0900107492,0.4420826355\O,2.2837635627,-1.0045755504,-0.3688935718\O,3.0066800731,-0.108004459,1.5711657172\C,3.8053094662,-1.2766701905,1.7541299383\H,1.445073105,1.7636633585,2.3606798698\H,0.7097542319,2.9092294018,1.2040468543\H,2.4720380217,2.726688769,1.311046336\H,4.3328706963,-1.1278902453,2.6945462152\H,4.5107035179,-1.3881017216,0.9278825266\H,3.1721064096,-2.1652876473,1.802558789\\Version=ES64L-G09RevD.01\State=2-A\HF=-690.488281\S2=0.75804\S2-1=0.\S2A=0.750048\RMSD=5.736e-09\RMSF=3.194e-06\Dipole=0.3714031,-0.6098358,0.6521283\Quadrupole=5.5090867,-2.709399,-2.7996877,4.9820097,1.6067424,-1.4469949\PG=C01 [X(C12H13O3)]\\@

T rad-MMA TS

1\1\GINC-R3398\Freq\UM062X\6-31+G(d,p)\C13H15O3S1(2)\ROOT\03-Jul-2014\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/6-31+G(d,p) Freq\\T_MMA_TS.freq\\0,2\C,0.0077288442,0.0072789419,0.0028734853\C,-0.0030073678,-0.003736667,1.4052371698\C,1.2148811209,-0.0267905917,2.1051172547\C,2.4171785388,-0.0401500337,1.4166907811\C,2.4260170025,-0.0273883955,0.0182982165\C,1.2155450544,-0.0034846591,-0.6827835912\H,-0.9179723542,0.0248701659,-0.560190912\S,-1.4680339592,0.0105435286,2.3850847299\H,1.2095578633,-0.0339969288,3.1910174273\H,3.3558112357,-0.0570541837,1.9613124301\C,3.7021077877,-0.0418900895,-0.7288154482\H,1.2343124766,0.0064821625,-1.7685323677\O,3.8698530328,0.0006584807,-1.9007900376\C,5.7232026288,-0.2330053274,0.4916152701\C,6.6337481789,-0.3065788101,-0.5109841142\H,5.3764394224,-1.1425683622,0.9754934675\H,5.5178937707,0.7118362543,0.9833633684\C,7.0378030706,-1.5872732476,-1.1745084687\C,7.1914147136,0.9230891997,-1.1134635338\O,8.013721732,0.9280546201,-2.0064023489\O,6.6966339773,2.0602743368,-0.5784446692\C,7.2096686222,3.2638898621,-1.1453198375\H,8.1261540791,-1.6653848988,-1.2457530831\H,6.6496493388,-1.6211281441,-2.199065551\H,6.649784747,-2.4469021394,-0.6237501525\H,6.7145686826,4.0752959467,-0.6141130575\H,6.983804779,3.3069846812,-2.2130058154\H,8.2922892349,3.3179360997,-1.0101806315\C,-2.7838350145,0.0447741195,1.1459541845\H,-3.7172786305,0.0567523915,1.7102368446\H,-2.730935302,0.9467338272,0.5332273308\H,-2.7635034452,-0.847705939,0.5176027878\\Version=ES64L-G09RevD.01\State=2-A\HF=-1127.8849806\S2=0.774221\S2-1=0.\S2A=0.750169\RMSD=3.257e-09\RMSF=9.725e-07\ZeroPoint=0.2525915\Thermal=0.271279\Dipole=-2.2731517,0.1029632,0.9948471\PG=C01 [X(C13H15O3S1)]\\@

T rad-MMA

1\1\GINC-R361\FOpt\UM062X\6-31+G(d,p)\C13H15O3S1(2)\ROOT\06-Mar-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=536870912\\T_MMA_rad.6a.freq\\0,2\C,-0.0293777082,-0.0474125471,-0.0030547695\C,-0.0518813197,-0.0696183767,1.4034447979\C,1.1563479514,-0.0461228142,2.1055179944\C,2.3676231866,-0.0045644909,1.4169917479\C,2.3900752328,0.0184897199,0.0204654876\C,1.1745541675,-0.0027163816,-0.6809735129\H,-0.9649722767,-0.0656048656,-0.5547443979\H,1.1736496152,-0.0613776927,3.1887766052\H,3.2894422512,0.0168333758,1.9914854075\C,3.655295711,0.066416549,-0.7653472085\H,1.2013023017,0.0161098716,-1.7657811037\O,3.6444246394,0.1117852356,-1.9809615797\C,4.9951497263,0.1166675501,-0.0207865734\C,5.279653484,1.5190692969,0.4119144879\H,5.7470105594,-0.2043573667,-0.7507119651\H,5.0102075314,-0.5550329315,0.8394716386\C,5.4840853418,2.5875548319,-0.606804362\C,5.4213438986,1.7919651238,1.8337680457\O,5.2663484886,0.9670755559,2.7231331259\O,5.752383345,3.0758826939,2.0861807927\C,5.9042130049,3.4022914917,3.4669952489\H,5.0252347315,3.5292857837,-0.2955952767\H,5.0783002393,2.280817668,-1.5737654226\H,6.5567022314,2.7887019232,-0.7370224382\H,6.1736274613,4.4566483824,3.492042224\H,6.689200448,2.7914257927,3.9179776841\H,4.9683329147,3.2299091957,4.0031324425\S,-1.6438928629,-0.1282899944,2.1620402992\C,-1.2471434485,-0.1464370224,3.925463534\H,-2.2064276431,-0.1843043869,4.4434110504\H,-0.6656562914,-1.0307119567,4.1935842608\H,-0.7197258913,0.761548975,4.2244576011\\Version=ES64L-G09RevD.01\State=2-A\HF=-1127.9394798\S2=0.758026\S2-1=0.\S2A=0.750048\RMSD=9.031e-09\RMSF=2.245e-06\Dipole=0.0922934,0.6401611,1.2114775\Quadrupole=2.6507776,-0.9773608,-1.6734168,4.3753384,-3.4413171,0.4618274\PG=C01 [X(C13H15O3S1)]\\@

D rad-MMA TS

1\1\GINC-R178\FTS\UM062X\6-31+G(d,p)\C14H19O4(2)\ROOT\28-Feb-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(2/17=4) Freq=noraman maxdisk=536870912\\MMA_rad_BenzylOCH32.TS.good5.SOLV.freq\\0,2\C,0.287339049,0.0315185227,-0.1496820346\C,0.1702326188,-0.0940213011,1.2044082759\C,2.4880698474,0.2194481564,-0.6492773962\H,0.1298586076,0.9931872674,-0.6259791261\H,0.2132305255,-0.8452564734,-0.7885067924\C,0.2251686409,-1.4073174644,1.9287781147\C,0.0776802918,1.0989350117,2.0710102543\O,-0.0091205,2.2605712818,1.3904121647\O,0.0569153449,1.0522302774,3.2867685469\C,-0.1279651434,3.4262581966,2.2007407457\H,-0.0087508294,-2.2346156998,1.2538971452\H,-0.4823043077,-1.4182026592,2.7613611447\H,1.2208820613,-1.577318433,2.3589283062\H,-0.1082691461,4.268088181,1.5096477704\H,0.7067689658,3.4880557556,2.9022504805\H,-1.0663538751,3.4042940507,2.7611675494\O,3.1113544603,-0.8333381811,-0.057301811\C,2.7734007387,1.5088415484,-0.0385880545\O,2.3372619625,0.1441510698,-2.005071464\C,3.1906940774,1.5830197737,1.3002682064\C,3.3709235589,2.8229423114,1.9046042432\C,3.1382584121,3.9982908241,1.1896349647\C,2.7135609283,3.9276854262,-0.1390794854\C,2.5263443128,2.6943950456,-0.7502888528\C,2.7567710575,-2.1351862049,-0.5030575958\C,3.5713142399,0.2199728233,-2.7317084513\H,3.3651582813,0.6668546495,1.8546083557\H,3.6894419583,2.8709300893,2.9415602444\H,3.2794536107,4.9634758497,1.6662725175\H,2.5242688415,4.8390868512,-0.6981318717\H,2.1725403719,2.6352528327,-1.7755846019\H,3.4767043112,-2.8139179602,-0.0470070057\H,2.8055576557,-2.2130905499,-1.5923386152\H,1.7482138496,-2.3909211815,-0.1660778347\H,3.3106571531,0.1391492285,-3.7867883213\H,4.2388703152,-0.6002956346,-2.4475482229\H,4.0706420266,1.174964765,-2.5386732898\\Version=ES64L-G09RevD.01\State=2-A\HF=-845.4198536\S2=0.776994\S2-1=0.\S2A=0.750377\RMSD=5.762e-09\RMSF=3.104e-06\Dipole=0.7257721,-0.2060487,-1.3430641\Quadrupole=-5.4358275,9.4777964,-4.0419689,-2.6243633,0.4286509,3.9847459\PG=C01 [X(C14H19O4)]\\@

D rad-MMA

1\1\GINC-R3305\FOpt\UM062X\6-31+G(d,p)\C14H19O4(2)\ROOT\06-Mar-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=536870912\\D_rad_MMA.2.freq\\0,2\C,-1.3074109157,-0.1241287166,-1.466843312\C,-0.747710704,1.2524163418,-1.3105120442\C,-2.3111803839,-0.5274338461,-0.3530169584\H,-0.5104167394,-0.8729358995,-1.4577449253\H,-1.8465901953,-0.1778333282,-2.4194107321\C,-1.4732825307,2.4239524338,-1.8728076794\C,0.4859327603,1.4878855777,-0.5697799909\O,1.0879739942,0.3453366612,-0.1707141933\O,0.9411060414,2.591361337,-0.3162551001\C,2.2241030594,0.5220701937,0.670941445\H,-1.530588418,2.3471392155,-2.9671385451\H,-0.9712886732,3.3551626999,-1.609018982\H,-2.5065435914,2.4368368786,-1.50614771\H,2.5517013441,-0.4818814809,0.9371286974\H,1.9423762529,1.0822589362,1.5660886312\H,3.0132318317,1.0619721656,0.1421778586\O,-3.4057922102,0.3495625926,-0.4983471331\C,-1.6674739559,-0.4120043442,1.0229623392\O,-2.7156098999,-1.866899374,-0.498638995\C,-1.6034211042,0.8367657492,1.6462425432\C,-0.9212486534,0.9878853036,2.8513980977\C,-0.3025671479,-0.1118456162,3.445726344\C,-0.3749966269,-1.3606081565,2.8310723627\C,-1.0552431676,-1.511465895,1.623182168\C,-4.5118790001,0.0715439467,0.3489254964\C,-3.293668818,-2.2134739302,-1.7451847199\H,-2.0849160222,1.692670802,1.1794075954\H,-0.8708218612,1.9645922809,3.3224213864\H,0.2306689318,0.0046040499,4.3843413646\H,0.099737578,-2.221465243,3.2921225697\H,-1.1112156006,-2.4794966706,1.1378376402\H,-5.2294528111,0.8761664231,0.1852071206\H,-4.2134462523,0.0532729763,1.4026330279\H,-4.9708512922,-0.8894978845,0.0941336553\H,-3.9878873988,-1.4393700894,-2.0910638117\H,-3.8397379116,-3.143616104,-1.5809764677\H,-2.5261699082,-2.3822099864,-2.5090690433\\Version=ES64L-G09RevD.01\State=2-A\HF=-845.462467\S2=0.758115\S2-1=0.\S2A=0.750048\RMSD=2.775e-09\RMSF=7.527e-06\Dipole=-0.5901252,-0.888765,-0.1311814\Quadrupole=1.9479228,-5.4968926,3.5489698,-4.6102273,5.0784153,3.0170376\PG=C01 [X(C14H19O4)]\\@

M rad-MMA TS

1\1\GINC-R556\Freq\UM062X\6-31+G(d,p)\C12H22N1O3(2)\ROOT\03-Jul-2014\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UM062X/6-31+G(d,p) Freq\\N_MMA_TS.freq\\0,2\C,1.1003573438,-1.5563249653,0.7109619469\C,0.480321573,-0.943848324,1.9583136582\N,1.3967851432,0.0244901,2.5621245921\C,2.7204625843,-0.5582020561,2.7861975801\C,3.2436598581,-1.1856685283,1.5019265006\O,2.3472454675,-2.1549964107,0.998363247\H,1.2310596546,-0.7807303835,-0.0605400345\H,0.4530287875,-2.3435852845,0.317494731\H,0.2517835659,-1.7415387029,2.682717744\H,-0.4477096969,-0.4437654803,1.6752682974\H,2.6819482697,-1.328076395,3.5713621845\H,3.4172408102,0.2202072109,3.1002293166\H,4.1897349231,-1.6967531928,1.6940516229\H,3.4050665581,-0.

4020733307,0.7444878372\C,0.8843749035,0.9214803334,3.498810146\C,-0.4455215229,1.5429709963,3.16431363\C,1.8817345345,1.7994961498,4.198896984\H,-0.4276818628,2.0151561796,2.1701850098\H,-0.6846250087,2.3168429569,3.8967802413\H,-1.2711984036,0.8232613373,3.1743746674\H,2.4562691512,2.4133144151,3.487085929\H,2.5917851496,1.2210237019,4.7974960867\H,1.3604037524,2.477686782,4.8783918814\C,0.1429108581,-0.3323738,5.387445057\H,-0.4783699355,-0.9043267163,4.7067936404\H,-0.2669758175,0.6018577315,5.7628185573\C,1.18234109,-0.9252204415,6.0399528037\C,1.6587585279,-2.2576691075,5.6482065601\C,1.9714317856,-0.258663289,7.1319470409\O,2.6496932429,-2.7960370124,6.1064027109\O,0.9112642121,-2.8442671093,4.6789119386\C,1.412578226,-4.0888787973,4.1954395166\H,3.0321472114,-0.181768654,6.8684780331\H,1.9270402109,-0.8408870424,8.0583279841\H,1.5825872783,0.7436047342,7.3292675139\H,0.6957438598,-4.4258011462,3.4472134324\H,1.4929060909,-4.8123848037,5.009205027\H,2.3959141689,-3.9514866604,3.737686236\\Version=ES64L-G09RevD.01\State=2-A\HF=-750.5717413\S2=0.767249\S2-1=0.\S2A=0.750094\RMSD=1.116e-09\RMSF=1.880e-06\ZeroPoint=0.3340203\Thermal=0.3520011\Dipole=-0.6817181,1.0563845,-0.9642637\PG=C01 [X(C12H22N1O3)]\\@

M rad-MMA

1\1\GINC-R1401\FOpt\UM062X\6-31+G(d,p)\C12H22N1O3(2)\ROOT\06-Mar-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=536870912\\N_MMA_rad.4.freq\\0,2\C,-3.9233449084,-0.483688234,-0.6169225304\C,-2.4584646794,-0.9000057041,-0.6391478756\N,-1.725974477,-0.1724728933,0.3944151059\C,-1.8674637086,1.2606514652,0.1417040607\C,-3.3446991687,1.6327231174,0.1400175419\O,-4.0627302096,0.9049096227,-0.8365551882\H,-4.363694019,-0.7546373719,0.3556027464\H,-4.4771769191,-0.9848048271,-1.414632324\H,-2.0580957768,-0.6983513227,-1.6499281703\H,-2.4016348409,-1.9754180856,-0.4552836117\H,-1.4286297421,1.5581689266,-0.8281014303\H,-1.3722786956,1.8316295952,0.9289832888\H,-3.4721615845,2.690679766,-0.1012157794\H,-3.7691307414,1.4351312967,1.136965301\C,-0.3542133529,-0.65350144,0.6657660663\C,-0.4334537913,-2.104187632,1.1607515997\C,0.2595016409,0.1922473088,1.7888911412\H,-1.1683094461,-2.1724806217,1.9686207823\H,0.5381484053,-2.4229397815,1.5480963886\H,-0.7150899094,-2.8078361111,0.3722737346\H,-0.4553403484,0.2783408409,2.6134688682\H,0.5538816851,1.1878423883,1.4503873693\H,1.1636063705,-0.2948474469,2.1662473995\C,0.5428263165,-0.5654876159,-0.6190020729\H,0.4879671214,0.4610033523,-0.9955426789\H,0.1201861843,-1.2399757605,-1.374245867\C,1.9729018337,-0.9183800854,-0.4064766548\C,2.9101435383,0.165382037,-0.1562367163\C,2.4664015069,-2.3275241105,-0.4613350861\O,2.6208089927,1.3514501961,-0.1194846618\O,4.1769081983,-0.2762383258,0.0371655257\C,5.1409205848,0.746304732,0.2789829651\H,2.8961789836,-2.6394517442,0.4989488549\H,3.2713981733,-2.4296176697,-1.1983529955\H,1.6597792643,-3.0159803569,-0.7210950847\H,6.0918320772,0.2316579415,0.4071267109\H,4.8824347338,1.3090445465,1.1788534207\H,5.1860507081,1.4357700075,-0.5670701439\\Version=ES64L-G09RevD.01\State=2-A\HF=-750.6074051\S2=0.758049\S2-1=0.\S2A=0.750046\RMSD=5.317e-09\RMSF=4.418e-06\Dipole=0.6748645,-0.9234144,0.2689858\Quadrupole=0.3472203,0.5415635,-0.8887838,1.734399,-1.4355954,3.0950452\PG=C01 [X(C12H22N1O3)]\\@

B rad/$AlCl_3$-MMA TS

1\1\GINC-R132\FTS\UM062X\6-31+G(d,p)\C12H13Al1Cl3O3(2)\ROOT\26-Jan-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(2/17=4) Freq=noraman maxdisk=536870912\\B_MMA_AlC3_TS.1.freq\\0,2\C,-4.2259610096,0.4195464842,0.3488672413\C,-4.8916244343,-0.7978532809,0.5089748338\C,-4.2491569634,-2.0072833386,0.2357680572\C,-2.9305003354,-2.0011600377,-0.1979946444\C,-2.2535524989,-0.7811019747,-0.3371921244\C,-2.9041006356,0.4380072099,-0.0742254522\H,-4.7375932643,1.3531312516,0.5555266598\H,-5.9239393489,-0.8035275399,0.8447173488\H,-4.7785854013,-2.9459604674,0.3562044223\H,-2.417169636,-2.9295098016,-0.4258581403\C,-0.8799142485,-0.7824936931,-0.8143134775\H,-2.383199537,1.3805036432,-0.2126897067\O,-0.1152068488,0.1558560764,-0.9009226252\C,0.3489218777,-2.7897855299,-0.6021869832\C,1.6110863365,-2.334930294,-0.7824521018\H,-0.1605035221,-3.3151459721,-1.405234958\H,-0.0773950614,-2.8413163282,0.3959452302\C,2.3445077446,-2.3548402899,-2.0838697892\C,2.3649469613,-1.7430168253,0.3641498042\O,3.5711455404,-1.7390367423,0.4337510761\O,1.5559331396,-1.2278365552,1.3034495177\C,2.2292761634,-0.6756368921,2.4444888802\H,3.3075758069,-2.8591419384,-1.9633483199\H,2.5662248112,-1.3290743179,-2.4017293929\H,1.7614062726,-2.8548544295,-2.8591360994\H,1.4409196166,-0.3479650687,3.1178002746\H,2.8440048157,0.1712037503,2.1314662384\H,2.8601631678,-1.4375718989,2.906278107\Al,0.5569743619,1.7796918085,-0.226926454\Cl,-0.1368440754,1.7866596317,1.7802122599\Cl,2.6359581289,1.5471434994,-0.4859825112\Cl,-0.4194859242,3.1977248609,-1.4586881711\\Version=ES64L-G09RevD.01\State=2-A\HF=-2313.5872417\S2=0.772668\S2-1=0.\S2A=0.750178\RMSD=7.494e-09\RMSF=3.069e-06\Dipole=-2.9427607,-2.4318237,0.0633874\Quadrupole=5.353785,-3.6997945,-1.6539905,4.9595581,-1.6046589,4.0669332\PG=C01 [X(C12H13Al1Cl3O3)]\\@

B rad/$AlCl_3$-MMA

1\1\GINC-R3290\FOpt\UM062X\6-31+G(d,p)\C12H13Al1Cl3O3(2)\ROOT\06-Mar-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=536870912\\B_MMA_rad_AlCl3.6.freq\\0,2\C,-2.7848885483,3.3115741807,0.6998872498\C,-2.3446056446,4.2042386934,-0.2781925301\C,-1.0191536228,4.1781514841,-0.713975182\C,-0.1247531086,3.2705602366,-0.1606300777\C,-0.5616409416,2.3754700607,0.8250181207\C,-1.9001163128,2.3906551412,1.2454253794\H,-3.8168946203,3.332163465,1.0328622285\H,-3.0387166625,4.9197260651,-0.7078815606\H,-0.6867576971,4.8600834651,-1.4890888426\H,0.8937108752,3.2285209659,-0.5304704022\C,0.3451470149,1.3978691001,1.4388014516\H,-2.2257833135,1.6834009533,2.0014077559\O,-0.171332923,0.4443017964,2.0581076337\C,1.8420642088,1.5879818049,1.4826114016\C,2.6066444963,0.4069297609,0.958360536\H,2.091300886,1.7435362847,2.5413063336\H,2.1250516497,2.5006119699,0.9474595238\C,3.8893713106,-0.0113445405,1.5772580814\C,2.0339751913,-0.2074423497,-0.2306822783\O,0.9754825022,0.1812492144,-0.7126244196\O,2.750321247,-1.2132944212,-0.7354844737\C,2.119186517,-1.9373367022,-1.7958620011\H,3.7181726468,-0.3355855791,2.6116042015\H,4.5934104942,0.8303047152,1.6172628763\H,2.8225568781,-2.7195514519,-2.0734353481\H,1.9179603478,-1.2754488204,-2.640321643\H,1.1818817482,-2.3682266013,-1.4369462266\Al,0.242883699,-0.9633613532,3.1901821019\Cl,-1.6287971185,-1.4371885056,4.0424415173\Cl,1.0975959503,-2.4585165184,1.9458358893\Cl,1.64

38090999,-0.1071046287,4.558140633\H,4.3417137502,-0.8316178857,1.0211620705\\Version=ES64L-G09RevD.01\State=2-A\HF=-2313.6566636\S2=0.757367\S2-1=0.\S2A=0.750042\RMSD=1.790e-09\RMSF=3.821e-06\Dipole=0.5535865,2.6963199,-2.3593835\Quadrupole=4.9424851,3.6145796,-8.5570647,-7.3410447,0.5288001,1.7887419\PG=C01 [X(C12H13Al1Cl3O3)]\\@

T rad/$AlCl_3$-MMA TS

1\1\GINC-R180\FTS\UM062X\6-31+G(d,p)\C13H15Al1Cl3O3S1(2)\ROOT\21-Feb-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=50,maxstep=5) IOP(2/17=4) Freq=noraman maxdisk=671088640\\T_MMA_AlCl3.2.freq\\0,2\C,0.0634254764,-0.374451177,0.0128535194\C,-0.0638418788,0.3991822661,1.1787526629\C,1.0845081847,0.9679660883,1.7672344905\C,2.3251095695,0.7723476349,1.1976500575\C,2.4491266781,0.0198009096,0.0152430157\C,1.3069174183,-0.5622743281,-0.5655706415\H,-0.8022177995,-0.8319445798,-0.4498490032\H,0.9862859261,1.5584010609,2.6727959741\H,3.2093525017,1.204252916,1.6548625868\C,3.7498609131,-0.1919515737,-0.5674570116\H,1.3968835873,-1.1725208847,-1.4594793836\O,4.0318099752,-0.7310880895,-1.6230443151\C,5.4981065465,1.2761252367,0.0581324863\C,6.4066652225,1.0138839273,-0.9102984077\H,5.6287559811,0.8622853761,1.054235363\H,4.7677647782,2.0691808995,-0.0760858207\C,7.5362688284,0.0449027242,-0.7764740371\C,6.3067509681,1.6961520696,-2.2354536587\O,7.2551956705,1.8806464775,-2.9613351327\O,5.0542267577,2.0847619322,-2.5233974557\C,4.9067796263,2.7756510386,-3.7721802484\H,8.4826216471,0.5346899437,-1.0229348837\H,7.4106306839,-0.7739141871,-1.494935255\H,7.5866092326,-0.3664866405,0.2332097618\H,3.8554271601,3.0466988808,-3.832805416\H,5.1802090299,2.109830698,-4.5936835057\H,5.5494312709,3.6582152955,-3.7851344328\Al,3.5990734644,-0.9966422573,-3.4268623526\Cl,2.2090810381,0.5617617106,-3.8272245426\Cl,5.4721633495,-0.8327375368,-4.3805711138\Cl,2.6987482461,-2.915676476,-3.3991281593\S,-1.5845471083,0.7137711003,1.9880565994\C,-2.7919527025,-0.1400355142,0.9471184399\H,-3.7602405237,0.0459601929,1.4133927139\H,-2.802314887,0.2693864041,-0.064452489\H,-2.6104198327,-1.2159865386,0.9275865955\\Version=ES64L-G09RevD.01\State=2-A\HF=-2751.0409048\S2=0.773736\S2-1=0.\S2A=0.750213\RMSD=2.757e-09\RMSF=2.455e-06\Dipole=-2.1729362,0.8188096,3.2340605\Quadrupole=10.1045678,-6.6794152,-3.4251526,0.8231524,2.0881467,-3.5898253\PG=C01 [X(C13H15Al1Cl3O3S1)]\\@

T rad/$AlCl_3$-MMA

1\1\GINC-R81\FOpt\UM062X\6-31+G(d,p)\C13H15Al1Cl3O3S1(2)\ROOT\05-Jun-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=1342177280\\T_rad_MMA.AlCl3.2.freq\\0,2\C,0.0092692012,0.0339642961,-0.0114118767\C,-0.0164117347,-0.0413814738,1.3891367832\C,1.1979172272,-0.1141301516,2.0974969027\C,2.4026737853,-0.1289175003,1.4226738799\C,2.4317023641,-0.0609411158,0.0190283758\C,1.2209827766,0.0334283394,-0.6837267744\H,-0.9085852647,0.0944950965,-0.5831714409\S,-1.4826731635,-0.0472433251,2.353314358\H,1.1841338797,-0.1502237973,3.1824360102\H,3.3228496149,-0.1502697684,1.9955227164\C,3.675039718,-0.0683553844,-0.74083235\H,1.243684405,0.0971911365,-1.7670478689\O,3.6148487861,0.23824785,-1.9541900372\C,4.9837575059,-0.5623077044,-0.1733403967\C,6.1118136993,0.4161044874,-0.3316465787\H,5.2205820421,-1.4809648104,-0.7274735059\H,4.8644389948,-0.8429568206,0.8782878357\C,7.4893347905,-0.0518862612,-0.6280324492\C,5.7584694076,1.8069518002,-0.0859420124\O,4.6100469092,2.149669772,0.1706052965\O,6.7828267611,2.6597593639,-0.1669333607\C,6.4278361008,4.043481614,-0.0992181079\H,7.5239287637,-0.5058916175,-1.6268464211\H,7.7974767635,-0.8265291301,0.0862135082\H,7.364218742,4.5896356828,-0.1925256156\H,5.9399779056,4.2646935193,0.852022458\H,5.7527384232,4.2887461004,-0.922169048\Al,4.604934433,0.2515376979,-3.5115610019\Cl,3.1177579345,0.3873500116,-5.0066249943\Cl,5.9032162215,1.9276914964,-3.3565281287\Cl,5.6437276286,-1.6169550695,-3.4731141019\H,8.1991732423,0.7736524019,-0.5930876076\C,-2.789866421,0.0859509058,1.111169376\H,-3.725432053,0.0936695352,1.6718094763\H,-2.7081686413,1.0170352731,0.5475216544\H,-2.788657004,-0.7735013981,0.4383883749\\Version=ES64L-G09RevD.01\State=2-A\HF=-2751.1094237\S2=0.757414\S2-1=0.\S2A=0.750042\RMSD=3.309e-09\RMSF=6.645e-06\Dipole=-1.4304529,-0.187197,3.3053654\Quadrupole=20.2653967,-3.3666088,-16.8987879,3.354156,4.9105871,-3.0221996\PG=C01 [X(C13H15Al1Cl3O3S1)]\\@

D rad/$AlCl_3$-MMA TS

1\1\GINC-R47\FTS\UM062X\6-31+G(d,p)\C14H19Al1Cl3O4(2)\ROOT\10-Jun-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(2/17=4) Freq=noraman maxdisk=2013265920\\D_rad_AlCl3_MMA.TS.1.freq\\0,2\C,-0.518151019,-1.4021591609,-0.8671223891\C,-1.7165587906,-1.9425425129,-0.4885744261\C,0.0472230536,-0.1584633352,0.9503899494\H,-0.5014000605,-0.5392486506,-1.5230326576\H,0.3805191521,-2.0136565718,-0.8314788686\C,-1.8529408135,-3.2153044285,0.2880116224\C,-2.9878983034,-1.2309825374,-0.7704164478\O,-2.8299860806,-0.1190196937,-1.5093571413\O,-4.0730032918,-1.6219668806,-0.3885762682\C,-4.0353063293,0.5689734064,-1.839052889\H,-0.9363798482,-3.8068226725,0.2330897945\H,-2.6887419582,-3.8103546865,-0.0879213018\H,-2.0702505308,-3.0008926007,1.3430599381\H,-3.7234758666,1.4749625732,-2.35638\H,-4.5919061093,0.814268326,-0.9322230319\H,-4.6585561906,-0.0535148937,-2.4858530413\O,-0.0982494867,-0.9980179392,1.9922887037\C,-0.9756285618,0.8958041495,0.8918285246\O,1.3995904001,0.3485690034,0.8681404284\C,-2.2063443319,0.6938663167,1.5312801639\C,-3.2082926323,1.6535920093,1.4254628248\C,-2.9934275178,2.8147454424,0.6835975852\C,-1.7700636114,3.0136685377,0.0428429915\C,-0.7634139762,2.0593460179,0.1416637885\C,0.8314958511,-2.0730991832,2.1244274511\C,1.7796958314,1.153112336,2.0426589103\H,-2.3721566538,-0.2142892995,2.10148049\H,-4.1606020336,1.4886111594,1.9196523507\H,-3.7781200456,3.5603514826,0.6006927916\H,-1.5994962454,3.9126415556,-0.5406226773\H,0.1762182969,2.207265523,-0.382178505\H,0.4763788641,-2.6658117143,2.9659993046\H,1.8375771431,-1.6950090648,2.3285386596\H,0.8560996837,-2.6778480995,1.2158400457\H,2.7612367636,0.8149994905,2.3688756175\H,1.0273307046,0.9804800618,2.8103237581\H,1.8084751788,2.1999030843,1.7428385774\Al,2.6579352428,0.1145006099,-0.5648765584\Cl,4.2672198913,1.3376641621,0.0693751263\Cl,3.10400149,-1.9581682473,-0.5424432328\Cl,1.7049507418,0.8352839251,-2.3084659616\\Version=ES64L-G09RevD.01\State=2-A\HF=-2468.5748592\S2=0.780401\S2-1=0.\S2A=0.750319\RMSD=3.091e-09\RMSF=2.363e-06\Dipole=-1.173382,0.6040252,1.7337532\Quadrupole=-12.9623873,7.3141263,5.648261,-8.8855918,8.2793772,-2.4412841\PG=C01 [X(C14H19Al1Cl3O4)]\\@

D rad/$AlCl_3$-MMA

1\1\GINC-R263\FOpt\UM062X\6-31+G(d,p)\C14H19Al1Cl3O4(2)\ROOT\24-Jun-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=671088640\\D_rad_MMA.AlCl3.r.13.freq\\0,2\C,-0.6952295112,-0.6302251827,-0.6859692917\C,-2.1759403166,-0.561664871,-0.8988357297\C,-0.2739408061,0.1954471799,0.5442225309\H,-0.1881764612,-0.2170504381,-1.5616917782\H,-0.3787546231,-1.6699112155,-0.5639019897\C,-2.8092665593,0.5089371522,-1.7232296621\C,-2.9938539573,-1.6190875518,-0.3199457903\O,-4.3111759078,-1.4353046325,-0.5454670503\O,-2.5592296429,-2.5807945098,0.2934700321\C,-5.1635459169,-2.4529276633,-0.0187960826\H,-2.0692492093,1.230004025,-2.0749108208\H,-3.5732695817,1.0458573844,-1.1497759954\H,-3.3225163984,0.0719855297,-2.5887525157\H,-6.1755263308,-2.1585311063,-0.290645107\H,-5.0564998169,-2.5131682441,1.0663756548\H,-4.9116292911,-3.4218319517,-0.4549333056\O,-0.786132576,-0.2779766913,1.729531686\C,-0.6769608421,1.6505524445,0.3833292719\O,1.2157169763,0.1511645166,0.6371936553\C,-1.7768051689,2.1602158811,1.0705146422\C,-2.1892471282,3.4731034627,0.8409615555\C,-1.5033413182,4.2755075761,-0.0677285661\C,-0.3954049817,3.7667374057,-0.7470598161\C,0.0151750268,2.4557333479,-0.5253955173\C,-0.3471298269,-1.5701399443,2.1672645168\C,1.7219899918,0.941823842,1.76017922\H,-2.3060408723,1.5257670473,1.7735132218\H,-3.0482374958,3.867140979,1.3746495542\H,-1.8260642371,5.2966271672,-0.2438787664\H,0.1501013079,4.389747957,-1.4482337109\H,0.8847902737,2.0647262233,-1.0508388942\H,-0.9140324671,-1.7699301548,3.0754207986\H,0.7241707228,-1.5530089227,2.3921443671\H,-0.5750490613,-2.3413632014,1.4309241293\H,1.9512553008,1.9462195636,1.4066756277\H,2.6183395926,0.4420941689,2.1270694406\H,0.9542624585,0.9544025018,2.5321724843\Al,2.6653333386,-0.6436533207,-0.3485060043\Cl,3.8533947685,1.087370919,-0.6815948712\Cl,2.0680692747,-1.5631447291,-2.1539983165\Cl,3.4111732734,-2.0067949435,1.096928193\\Version=ES64L-G09RevD.01\State=2-A\HF=-2468.6205548\S2=0.758178\S2-1=0.\S2A=0.750048\RMSD=5.409e-09\RMSF=5.348e-06\Dipole=-2.8122089,1.53375,0.8116441\Quadrupole=-4.2796437,2.2099441,2.0696996,3.9323323,3.5209971,-0.8338795\PG=C01 [X(C14H19Al1Cl3O4)]\\@

Nbound M rad/$AlCl_3$-MMA TS

1\1\GINC-R54\FTS\UM062X\6-31+G(d,p)\C12H22Al1Cl3N1O3(2)\ROOT\07-Mar-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(2/17=4) Freq=noraman maxdisk=671088640\\M_rad_AlCl3_TS.2.freq\\0,2\C,2.1471558754,-1.7669372745,0.9698622679\C,3.0121736576,-1.3586559916,-0.0162811346\C,3.5629543565,0.0149212698,-0.0564692365\O,4.1077539851,0.4832049363,-1.0356546697\O,3.4037356825,0.7029326336,1.0903506902\C,3.8620401565,2.0602818969,1.0498843009\C,3.3891793122,-2.2176554119,-1.1875755493\H,2.0583210138,-1.1929593849,1.8862082997\H,1.9276926696,-2.8279226771,1.0481332371\H,3.6859679503,2.4562667718,2.049156046\H,3.295806418,2.6161139205,0.2993380837\H,4.9259416893,2.0892290991,0.8078249824\H,3.0070917982,-3.2333912752,-1.0661096129\H,4.4773812252,-2.2574723055,-1.297020826\H,3.0092162521,-1.8031089868,-2.1299328629\C,-0.0210901118,-1.547472421,0.4102608215\C,-0.6013223955,-1.994883782,1.7264588029\C,-0.0453731575,-2.5610411762,-0.7056042954\N,-0.36273995,-0.1472342457,0.020726765\C,0.1707803415,0.8108914028,1.0647375839\C,0.2898750178,0.170908713,-1.3103334788\H,-0.1508743149,-2.9513124838,2.0033970821\H,-1.6845160151,-2.1617829432,1.6583977736\H,-0.4204384481,-1.2912369363,2.5413704718\H,0.1157758237,-3.552813887,-0.2759079318\H,0.7362154345,-2.3888061135,-1.4479120985\H,-1.009663253,-2.5868490423,-1.2219205663\H,-0.4237527359,0.7114619452,1.9700777985\C,0.163289572,2.2477994821,0.5816453924\H,1.2059131237,0.5412362691,1.2672803414\H,-0.2957168717,-0.3055221059,-2.1022553104\H,1.2824243172,-0.2824019001,-1.2893403202\C,0.4555141084,1.6586397736,-1.6260843611\Al,-2.4391877975,0.0586876613,-0.0588728099\Cl,-2.9839605813,0.6712855813,1.9075590512\Cl,-2.9207648308,1.5103478076,-1.5336611744\Cl,-3.3302349227,-1.8007320188,-0.5817382502\O,1.0116612133,2.3716445038,-0.5410585805\H,0.5736307535,2.8800523188,1.3729530842\H,-0.8492538314,2.6072865601,0.3436303472\H,-0.4902690381,2.1171388894,-1.9246343135\H,1.1640475073,1.7342479273,-2.4542958406\\Version=ES64L-G09RevD.01\State=2-A\HF=-2373.7260963\S2=0.782128\S2-1=0.\S2A=0.750244\RMSD=4.201e-09\RMSF=3.719e-06\Dipole=2.0607827,-0.7983432,0.6738422\Quadrupole=-16.6203717,10.4345585,6.1858132,-1.3358527,4.0631144,2.7196877\PG=C01 [X(C12H22Al1Cl3N1O3)]\\@

Nbound M rad/$AlCl_3$-MMA

1\1\GINC-R1263\FOpt\UM062X\6-31+G(d,p)\C12H22Al1Cl3N1O3(2)\ROOT\06-Mar-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=671088640\\N_MMA_rad_AlCl3.2.freq\\0,2\C,-8.0260775892,1.9452819112,0.6622488696\C,-7.387249666,0.5882786907,0.9010024873\N,-5.9400557512,0.6989208405,1.3200736104\C,-5.2408895174,1.6413096668,0.3581314771\C,-6.0435241531,2.8796734294,-0.0587947506\O,-7.3722804858,2.5695924722,-0.4231580988\H,-8.0082428219,2.5884589463,1.5531654597\H,-9.067339123,1.79266236,0.3705476461\H,-7.4395091137,0.0683247483,-0.0551582621\H,-7.9308813937,0.0203082436,1.6546402051\H,-4.9892301345,1.0739525221,-0.542119953\H,-4.3053597432,1.9684330935,0.8208785968\H,-5.5580310396,3.2931924804,-0.9458827635\H,-6.0428886913,3.6396660211,0.7247875359\C,-5.2601904666,-0.7052050607,1.2186696848\C,-5.7377019321,-1.5929622 6,2.3720302578\C,-3.7354731643,-0.5415414338,1.2770286477\H,-5.3650300854,-1.2601860925,3.3424806406\H,-5.3454947466,-2.6003913387,2.209010514\H,-6.8271351703,-1.6653867034,2.4179968398\H,-3.4240446354,0.0895352548,2.1075248685\H,-3.3275155978,-0.1458946647,0.3457542516\H,-3.2923052187,-1.5281794721,1.4428745574\C,-5.6601928327,-1.4095459288,-0.127325427\H,-5.7409754757,-0.6743492704,-0.9312527644\H,-6.6381453799,-1.8858019052,0.0047067356\C,-4.6904262094,-2.4486430628,-0.5897727589\C,-3.6932302053,-2.0189738169,-1.563063714\C,-4.7117307044,-3.8530018444,-0.088621984\O,-3.6110048029,-0.8825809142,-2.0064324513\O,-2.8532669847,-3.0060642392,-1.9303139784\C,-1.8590575884,-2.6341130402,-2.8872235296\H,-3.9522186492,-4.0071749135,0.6922778589\H,-4.475722912,-4.5592636327,-0.8883957901\H,-5.6856042827,-4.1021508522,0.3400707346\H,-1.2789321233,-3.5358592339,-3.0732509493\H,-1.2245513739,-1.8416425423,-2.4851321901\H,-2.3317118521,-2.2805105453,-3.805804928\Al,-5.9084742171,1.442601168,3.2667608332\Cl,-7.6902264368,0.667504406,4.151190696\Cl,-4.1624606975,0.8766065883,4.3538057503\Cl,-5.9331570311,3.5723299245,3.2196155341\\Version=ES64L-G09RevD.01\State=2-A\HF=-2373.7659113\S2=0.757879\S2-1=0.\S2A=0.750046\RMSD=2.952e-09\RMSF=1.099e-05\Dipole=0.498375,-2.3092081,-2.4115865\Quadrupole=6.7640552,4.9085034,-11.6725586,-0.7350566,-2.8284396,-0.9834895\PG=C01 [X(C12H22Al1Cl3N1O3)]\\@

Obound M rad/$AlCl_3$-MMA TS

1\1\GINC-R45\FTS\UM062X\6-31+G(d,p)\C12H22Al1Cl3N1O3(2)\ROOT\26-May-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(2/17=4) Freq=noraman maxdisk=2013265920\\M_rad_AlCl3_rad.Ob.2b.TS.freq\\0,2\C,3.905226147,0.0243078382,0.7958486569\C,3.536347568,1.1065026279,0.0510270001\C,2.3777312246,1.8849331224,0.5233975143\O,1.8105617776,1.7389651482,1.5933816597\O,1.9536832083,2.7771506335,-0.3946863973\C,0.7935166607,3.5288538758,-0.0241450464\C,4.1802210971,1.4764055653,-1.2564490758\H,3.4786683587,-0.1040406914,1.7862003576\H,4.8346883786,-0.4952743487,0.5794803269\H,0.5670925935,4.1629859359,-0.8790303617\H,1.0003455266,4.1278830067,0.8648731411\H,-0.0436003997,2.8584542571,0.1851191285\H,5.061842008,0.8553007495,-1.4349631685\H,4.4870992065,2.5265307045,-1.2642749275\H,3.4901533297,1.3516138421,-2.1007653233\C,2.8179848025,-1.9205408747,0.0465371094\C,3.1537530734,-2.8089882263,1.2142257338\C,3.6070924777,-2.1672027321,-1.2108303754\N,1.4598956718,-1.6185750572,-0.1295660156\C,0.7049597613,-1.2544152659,1.0732892487\C,1.1046556928,-0.79376298,-1.2829479898\H,4.2298808165,-2.9942824449,1.2343858862\H,2.6471939246,-3.7826481168,1.1288340721\H,2.8844155474,-2.3746028164,2.180745376\H,4.6289159624,-2.4522546397,-0.9513488134\H,3.669056668,-1.2819187105,-1.850430788\H,3.174196774,-2.9880521368,-1.8035088456\H,0.8525917295,-2.0203323726,1.8372078022\C,-0.7826056681,-1.1998247275,0.80119318\H,1.0394797061,-0.2867231851,1.4740812684\H,1.5600582893,-1.2089755794,-2.1838101326\H,1.4542245555,0.2429424336,-1.1688951374\C,-0.3899888414,-0.7801450577,-1.5063598379\O,-1.0367691408,-0.2867332579,-0.3032629728\H,-1.317783601,-0.7982838768,1.6620440227\H,-1.1958994065,-2.1730138184,0.5135814729\H,-0.7925702291,-1.7788061697,-1.7089080382\H,-0.6583840578,-0.0922753241,-2.3085936738\Al,-2.7167768732,0.5920970649,-0.4480644625\Cl,-3.0141031874,1.3670974715,1.4923572576\Cl,-2.3460437888,2.0231666784,-1.9643622413\Cl,-3.9547873441,-1.034798545,-1.0082965905\\Version=ES64L-G09RevD.01\State=2-A\HF=-2373.7387619\S2=0.769358\S2-1=0.\S2A=0.750107\RMSD=2.304e-09\RMSF=1.265e-06\Dipole=2.5136816,-1.7886339,-0.4539489\Quadrupole=-7.6434551,7.058118,0.5853371,-3.9920525,-4.1520351,-3.366184\PG=C01 [X(C12H22Al1Cl3N1O3)]\\@

Obound M rad/$AlCl_3$-MMA

1\1\GINC-R76\FOpt\UM062X\6-31+G(d,p)\C12H22Al1Cl3N1O3(2)\ROOT\22-Mar-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=1073741824\\M_rad_AlCl3_rad.Ob.2.freq\\0,2\C,-1.7004720469,1.7874768523,0.7870548385\C,-2.8671280295,1.4871600104,-0.0953202471\C,-3.7692092994,0.3671003617,0.1572212554\O,-4.7842465491,0.1611838797,-0.4843817011\O,-3.3766637953,-0.4300649045,1.1777343658\C,-4.2675902883,-1.5108359191,1.483018479\C,-3.2764291099,2.4020143285,-1.2032750641\H,-1.812453115,1.2589660019,1.7385576945\H,-1.7185882583,2.864039102,1.0115043097\H,-3.7928560881,-2.0625519722,2.2926749758\H,-4.39840147,-2.1515143775,0.6095674343\H,-5.2373398535,-1.1155335133,1.7936075168\H,-2.6748095679,3.3129470768,-1.2130198791\H,-4.3349086326,2.6656277406,-1.1047055813\H,-3.1841354711,1.911020595,-2.1811018341\C,-0.2637255698,1.4891035275,0.2351772263\C,0.7357329603,2.0794114252,1.2442536063\C,-0.0264967159,2.1985422765,-1.1025460443\N,0.0372575212,0.048810833,0.0770138494\C,-0.0701633597,-0.7544872944,1.2946179271\C,-0.622664849,-0.6543788228,-1.0205646266\H,0.6938641631,3.1712330244,1.2097488996\H,1.7511619881,1.7613106993,0.990839757\H,0.5185912618,1.7850132228,2.2744846804\H,-0.1028158435,3.2804513768,-0.9614254043\H,-0.7483630817,1.9235276022,-1.8733507625\H,0.9799011313,1.968097951,-1.466340529\H,0.445763981,-0.2579591879,2.1191656263\C,0.6087494006,-2.0915659639,1.0836248711\H,-1.1173452271,-0.9308542982,1.5913422034\H,-0.529965542,-0.0861400551,-1.9477291815\H,-1.6928853097,-0.8432520832,-0.8343121154\C,0.0579507456,-1.9903175568,-1.2450513815\O,-0.03352163,-2.7776401797,-0.0257871232\H,0.5095078652,-2.7429475027,1.9507253028\H,1.6609086088,-1.9732514451,0.8079253937\H,1.1235984452,-1.8709381558,-1.4614877136\H,-0.4287193988,-2.5702068449,-2.0291552508\Al,-1.203681216,-4.2615417979,0.1249250436\Cl,-1.7021492129,-4.263544906,2.187995884\Cl,-2.8009540997,-3.7258108077,-1.1655426344\Cl,-0.027384859,-5.880230299,-0.5458740671\\Version=ES64L-G09RevD.01\State=2-A\HF=-2373.7754419\S2=0.757803\S2-1=0.\S2A=0.750046\RMSD=4.539e-09\RMSF=1.525e-06\Dipole=1.7990086,2.856836,0.3114507\Quadrupole=-0.1351996,-4.9278741,5.0630737,4.3881075,-3.3859019,-0.9185246\PG=C01 [X(C12H22Al1Cl3N1O3)]\\@

B rad -MMA/$AlCl_3$ TS

1\1\GINC-R3080\FTS\UM062X\6-31+G(d,p)\C12H13Al1Cl3O3(2)\ROOT\26-Jan-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(2/17=4) Freq=noraman maxdisk=536870912\\B_MMA_AlC3_TS.1.MON.freq\\0,2\C,-3.8335161403,-0.8250676002,1.1271246051\C,-4.4966026485,-0.8124122598,-0.1016744038\C,-4.1791139438,0.1373436301,-1.0725737094\C,-3.1778532153,1.0683622297,-0.8223835963\C,-2.5266922293,1.0625853219,0.4129602606\C,-2.8504138974,0.118878272,1.3968926245\H,-4.0797654736,-1.5759249964,1.8705162571\H,-5.2600109392,-1.5561832732,-0.307331321\H,-4.6937897989,0.1347153545,-2.027325545\H,-2.8914421959,1.795825536,-1.5764306182\C,-1.43539699,2.0175808337,0.6606426104\H,-2.3110178049,0.121540745,2.338209486\O,-0.9270082158,2.4020105065,1.6537149128\C,0.1558820454,2.3537553301,-1.3328434351\C,1.3307884197,2.4745318757,-0.6716052201\H,-0.4252450826,3.236590688,-1.5777399517\H,-0.1701999942,1.3991966792,-1.7383217278\C,1.8459652546,3.7568790332,-0.0843449892\C,2.073655862,1.251893551,-0.4275309662\O,1.7243613184,0.1240590102,-0.8706145249\O,3.1736166119,1.3849996915,0.2613367762\C,3.9401033483,0.1980148669,0.5606854811\H,2.8677564209,3.9671159986,-0.4117095344\H,1.8507412694,3.7005482614,1.0086407174\H,1.2032078158,4.5867638695,-0.3822054102\H,4.865533278,0.5651763913,0.9966933557\H,4.1257150709,-0.3665055393,-0.3537211305\H,3.3897104247,-0.4145270328,1.2775927206\Al,0.8724235889,-1.3777629624,-0.2574233303\Cl,2.2727854466,-2.9527481254,-0.4788565645\Cl,0.5152680437,-0.8315882847,1.7815777036\Cl,-0.8877676493,-1.541599602,-1.4273105517\\Version=ES64L-G09RevD.01\State=2-A\HF=-2313.6116583\S2=0.76315\S2-1=0.\S2A=0.750066\RMSD=5.404e-09\RMSF=2.449e-06\Dipole=-0.0811559,2.0003167,-0.442144\Quadrupole=14.4938675,-8.0594026,-6.4344649,8.9825846,3.0407767,-7.5510338\PG=C01 [X(C12H13Al1Cl3O3)]\\@

B rad -MMA/$AlCl_3$

1\1\GINC-R3504\FOpt\UM062X\6-31+G(d,p)\C12H13Al1Cl3O3(2)\ROOT\06-Mar-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IO
P(2/17=4) Freq=noraman maxdisk=536870912\\B_MMA_rad_AlCl3.MON.2.freq\\0,2\C,-4.1742081396,0.0595298152,0.7290349159\C,-4.
5039406357,-0.4833997008,-0.5142990513\C,-3.5239423643,-0.6382068284,-1.4924206451\C,-2.2119342264,-0.2486011738,-1.234302
4178\C,-1.879202441,0.2978794098,0.0093749502\C,-2.8662955948,0.4472015099,0.9910733146\H,-4.9368468439,0.1753439086,1.49
22642263\H,-5.524802347,-0.7917030502,-0.71758058\H,-3.7748913409,-1.072959116,-2.4541624902\H,-1.4613039898,-0.4020147358,
-2.0027317871\C,-0.4951371701,0.7323481208,0.356953534\H,-2.5838336219,0.863829471,1.9522230996\O,-0.2028866093,1.1221868
627,1.4675063292\C,0.5597313788,0.7470242233,-0.7704128888\C,1.9341997235,0.9250031258,-0.2376044136\H,0.3029070261,1.606
5575266,-1.4080361962\H,0.4754294987,-0.1446331912,-1.3927688551\C,2.3323905618,2.1816230585,0.4485669286\C,2.8772458492,
-0.1530294807,-0.3439303269\O,2.6522598591,-1.2629235273,-0.8925933042\O,4.0742919172,0.0836550905,0.1461012186\C,5.02716
68281,-0.9974201317,0.0877074407\H,2.238793695,2.039881406,1.5333295036\H,1.6615487485,2.9972540312,0.1744665955\H,3.367
5013295,2.452756273,0.2289616023\H,5.9247743595,-0.606458392,0.5594757199\H,5.2113181756,-1.2706370599,-0.952081287\H,4.6
386290407,-1.8613692722,0.6292457476\Al,1.5332114747,-2.7148370868,-1.0245307635\Cl,2.861389553,-4.3592899841,-0.966369102
2\Cl,0.5091086554,-2.4290633508,-2.8693458817\Cl,0.2828776503,-2.4800377514,0.6798448642\\Version=ES64L-G09RevD.01\State=2-
A\HF=-2313.6574535\S2=0.754725\S2-1=0.\S2A=0.750019\RMSD=4.900e-09\RMSF=3.320e-06\Dipole=0.8041819,2.5764129,0.0572144\
Quadrupole=20.2544521,-10.7453658,-9.5090863,7.133271,3.5913234,-3.5894696\PG=C01 [X(C12H13Al1Cl3O3)]\\@

T rad -MMA/$AlCl_3$ TS

1\1\GINC-R546\FTS\UM062X\6-31+G(d,p)\C13H15Al1Cl3O3S1(2)\ROOT\21-Feb-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT=(T
S,calcfc,noeigentest,maxcyc=50,maxstep=5) IOP(2/17=4) Freq=noraman maxdisk=671088640\\T_MMA_AlCl3.2.MON.freq\\0,2\C,0.11279
5544,-0.0776722109,-0.0390907216\C,0.0919228497,0.0468187255,1.3629546579\C,1.2909731952,-0.0225164707,2.0833452707\C,2.49
30300497,-0.1791929047,1.4064685411\C,2.5093812338,-0.3033587218,0.0173835511\C,1.307113339,-0.2597493357,-0.7088632705\H
,-0.8166981493,-0.0106328802,-0.5966709079\H,1.2997834553,0.0711462629,3.1622846869\H,3.4291967223,-0.1994689133,1.957390
3038\C,3.7858334625,-0.4046210728,-0.6906559671\H,1.3337075585,-0.3344259605,-1.7908672607\O,4.0625835383,-0.7116998777,-1
.7978708003\C,5.5951944043,1.1519130155,0.2630765724\C,6.1685464509,1.5508947663,-0.8963165218\H,5.9921170936,0.29921012
73,0.8037235652\H,4.8145737091,1.7408301953,0.7380236837\C,7.2490699672,0.7932285123,-1.6123513323\C,5.6078858264,2.72867
12836,-1.532561189\O,4.6936908005,3.4274982146,-1.0175334275\O,6.1386087973,3.0596942281,-2.6777720342\C,5.6141664306,4.2
144094584,-3.368623283\H,8.103820095,1.434165816,-1.8446668048\H,6.8690493496,0.3884230293,-2.5555447159\H,7.590632888,-0
.0391454657,-0.9950599017\H,6.2980173899,4.3788304979,-4.1973105838\H,5.5893443905,5.0721229332,-2.6954505053\H,4.6096658
508,3.991206217,-3.7334879229\Al,2.8922246016,3.7125837987,-1.1872858537\Cl,2.6911098024,5.7491499499,-1.7423701005\Cl,2.40
62891442,2.3478898267,-2.7615878379\Cl,2.0642666875,3.2000442823,0.6965345946\S,-1.4875993935,0.2927305235,2.0976644837\C
,-1.0811255417,0.6008238035,3.831990679\H,-2.0298973079,0.8281362963,4.3198971938\H,-0.6437001687,-0.2795120953,4.3067819
454\H,-0.4169950668,1.4619171455,3.9300982132\\Version=ES64L-G09RevD.01\State=2-A\HF=-2751.0632408\S2=0.763133\S2-1=0.\S2
A=0.750069\RMSD=3.710e-09\RMSF=2.535e-06\Dipole=1.6444985,-1.117036,1.1047221\Quadrupole=9.0989317,-16.1667407,7.067809,
6.0034137,-9.9551858,-7.600513\PG=C01 [X(C13H15Al1Cl3O3S1)]\\@

T rad -MMA/$AlCl_3$

1\1\GINC-R66\FOpt\UM062X\6-31+G(d,p)\C13H15Al1Cl3O3S1(2)\ROOT\05-Jun-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IO
P(2/17=4) Freq=noraman maxdisk=1342177280\\T_rad_MMA.AlCl3.3.MON.freq\\0,2\C,0.0060788544,0.0932033224,0.0241123255\C,0.0
01327151,0.0332657002,1.4313024158\C,1.2190659271,-0.028501799,2.1152390316\C,2.4191959676,-0.0295716839,1.4089760718\C,2
.4254372383,0.0293394807,0.0130598595\C,1.1991741244,0.0896179055,-0.6713210296\H,-0.9368399997,0.1382712172,-0.513146505
2\S,-1.5773264432,0.039516296,2.211012513\H,1.2539233884,-0.0844564121,3.1966416993\H,3.3418915279,-0.0894822681,1.975485
8259\C,3.6712337532,0.0339698886,-0.7929079599\H,1.2099800681,0.1317255481,-1.7556463164\O,3.6562555568,0.0814398104,-2.0
065597289\C,5.0410571752,0.0469706806,-0.0716608917\C,5.4547881822,1.4680495542,0.0893026499\H,5.738755149,-0.4532616098,
-0.7505772969\H,5.0129580096,-0.4920239177,0.8754154292\C,5.8546333516,2.2505069948,-1.1090637176\C,5.5057444333,2.056991
1562,1.395021789\O,5.2824908041,1.4176104012,2.4678427588\O,5.7990150245,3.3336387522,1.4432829144\C,5.9728096282,3.9254
043221,2.7480867777\H,5.3134959204,1.8906237222,-1.9880748449\H,6.926240047,2.0844764316,-1.2927319076\H,5.7014968371,3.3
21511645,-0.9758394762\H,6.1488892476,4.9804373846,2.555957545\H,6.8298353223,3.4673482176,3.2453595295\H,5.0742708239,3
.7727962504,3.3465810711\Al,6.3307747856,0.2306333548,3.4144589933\Cl,6.7569895304,1.2053637189,5.2450476055\Cl,8.0003257
475,0.0637477891,2.0897147269\Cl,5.1433888243,-1.5197620201,3.5671895715\C,-1.1605773011,-0.1014459051,3.9646496208\H,-2.1
147931842,-0.119747327,4.4928178137\H,-0.6239766128,-1.0293096004,4.1713709721\H,-0.5832265888,0.7589124408,4.308329064\\
Version=ES64L-G09RevD.01\State=2-A\HF=-2751.1091145\S2=0.754636\S2-1=0.\S2A=0.750018\RMSD=4.267e-09\RMSF=2.423e-06\Dipol
e=-1.2776914,2.0287881,-0.6529226\Quadrupole=-1.8978524,7.0856553,-5.1878029,8.4311526,-14.4923685,-0.1883896\PG=C01 [X(C13
H15Al1Cl3O3S1)]\\@

D rad -MMA/$AlCl_3$ TS

1\1\GINC-R1734\FTS\UM062X\6-31+G(d,p)\C14H19Al1Cl3O4(2)\ROOT\06-Mar-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT=(TS
,calcfc,noeigentest,maxcyc=200) IOP(2/17=4) Freq=noraman maxdisk=671088640\\MMA_rad_AlCl3_BenzylOCH32.TS.good4.freq\\0,2\C,-
1.441922886,0.2051766117,-1.6317931786\C,-1.0316021052,1.4568117725,-1.2737352791\C,-2.8435878551,-0.4882065725,0.15712352
43\H,-0.8197075996,-0.6650034968,-1.4407226436\H,-2.264886304,0.0755459394,-2.328105452\C,-1.7930541976,2.7153390531,-1.580

1529635\C,0.1634965899,1.5507566805,-0.4722480375\O,0.5114082231,2.7577219266,-0.0875625708\O,0.8545176045,0.5530364432,-0.1314492779\C,1.7159737949,2.8799467217,0.6941418751\H,-2.6142202448,2.4993514117,-2.2668677278\H,-1.1483414631,3.4697526064,-2.0390846107\H,-2.2115533125,3.1541698218,-0.6673821677\H,1.746171586,3.9212571011,1.0059517224\H,2.5822178232,2.636763443,0.0745052382\H,1.6688416862,2.2071311489,1.5528190352\O,-3.7739230956,0.4865683545,0.220768993\C,-1.8257094357,-0.4572143154,1.1854677934\O,-3.2109565287,-1.6513305492,-0.4289803901\C,-1.630600038,0.7033972811,1.9545350625\C,-0.5736796213,0.764961719,2.8586745522\C,0.3023732564,-0.311717295,2.9950596097\C,0.1110422365,-1.4661323805,2.2302076215\C,-0.9429760876,-1.5430462226,1.3315431932\C,-4.7577795418,0.5288031887,-0.8069436305\C,-3.9904189083,-2.5207342957,0.4134394853\H,-2.3109167514,1.5409209581,1.8393852057\H,-0.4310799334,1.6614178329,3.4552615499\H,1.1444966218,-0.2505121158,3.6765248883\H,0.8101634021,-2.2926799039,2.3103225446\H,-1.0564345971,-2.4182252952,0.6982600553\H,-5.3876091121,1.3860717569,-0.5750579565\H,-5.3573394651,-0.3840577313,-0.8235977137\H,-4.2874181667,0.6662287081,-1.7848928247\H,-4.2514101827,-3.3811241769,-0.2009903695\H,-4.8978209014,-2.0114599065,0.7540383592\H,-3.4014531065,-2.8370304685,1.2787103086\Al,2.3391281921,-0.427876949,-0.47871568\Cl,3.4867473467,-0.389251403,1.3161152529\Cl,1.6341615021,-2.3635914249,-1.0168611166\Cl,3.2451815759,0.6542140216,-2.0792122795\\Version=ES64L-G09RevD.01\State=2-A\HF=-2468.6004131\S2=0.769738\S2-1=0.\S2A=0.750226\RMSD=5.998e-09\RMSF=3.383e-06\Dipole=-3.9981865,1.2598733,0.7257789\Quadrupole=0.2172522,4.9647194,-5.1819716,7.9829865,9.7202552,-0.6900624\PG=C01 [X(C14H19Al1Cl3O4)]\\@

D rad -MMA/$AlCl_3$

1\1\GINC-R2049\FOpt\UM062X\6-31+G(d,p)\C14H19Al1Cl3O4(2)\ROOT\06-Mar-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=671088640\\D_rad_MMA_AlCl3.1.freq\\0,2\C,-1.3272426145,-0.0654681128,-1.5151326242\C,-0.8343500502,1.3188228044,-1.2803003549\C,-2.3327043849,-0.5104982666,-0.4068709051\H,-0.5028545849,-0.7859808204,-1.5063136975\H,-1.8466726491,-0.1024723045,-2.4774612121\C,-1.6019065009,2.5192852807,-1.7107834112\C,0.3743422669,1.4916031955,-0.519186609\O,0.6939962697,2.7302414766,-0.2252004366\O,1.0652426519,0.5181148581,-0.1340412641\C,1.8455190315,2.9374482727,0.6196217992\H,-2.4874467328,2.2257464377,-2.2730049295\H,-0.9776159394,3.1856785574,-2.3167713307\H,-1.9234201455,3.1010848257,-0.8380479096\H,1.8594199598,4.0062401688,0.8182033436\H,2.7514171099,2.629513615,0.0931240962\H,1.7280899195,2.3630186775,1.5413675454\O,-3.4405029193,0.3473787454,-0.5550309198\C,-1.6605613846,-0.372257213,0.9525184936\O,-2.6939536216,-1.851606535,-0.558109698\C,-1.7028619351,0.8516712801,1.6248720541\C,-0.9171656543,1.0566063394,2.7596479496\C,-0.0796794612,0.0415280185,3.2198420167\C,-0.0536162597,-1.1872121514,2.5605811204\C,-0.8466660501,-1.3971380873,1.4343713061\C,-4.5559234787,0.0179612259,0.2650362113\C,-3.2240312173,-2.2218790527,-1.8211846243\H,-2.345558085,1.6457312879,1.2517282779\H,-0.9561495282,2.0103406591,3.277802046\H,0.5579105758,0.2068446722,4.0823956551\H,0.6088034407,-1.9750840069,2.9053191157\H,-0.8036317372,-2.3405683602,0.9010581354\H,-5.2690425052,0.8347542961,0.150437011\H,-4.2640106842,-0.0739906232,1.3164863544\H,-5.0152350574,-0.9215197433,-0.0578893282\H,-3.9444973355,-1.4797058592,-2.1832521132\H,-3.7292746161,-3.1763366838,-1.6709484386\H,-2.4273628576,-2.3549315446,-2.5615401376\Al,2.6245345945,-0.4222527466,-0.0113314109\Cl,3.3768902653,-0.0963237156,1.9512756637\Cl,2.0569776907,-2.4250450105,-0.4270606908\Cl,3.8141942143,0.4935861428,-1.5272261495\\Version=ES64L-G09RevD.01\State=2-A\HF=-2468.6374388\S2=0.754903\S2-1=0.\S2A=0.75002\RMSD=3.905e-09\RMSF=5.066e-06\Dipole=-3.150068,1.8623942,-0.3126515\Quadrupole=-7.8498511,5.7830397,2.0668114,5.2475829,7.4505733,2.7984695\PG=C01 [X(C14H19Al1Cl3O4)]\\@

M rad -MMA/$AlCl_3$

1\1\GINC-R1937\FOpt\UM062X\6-31+G(d,p)\C12H22Al1Cl3N1O3(2)\ROOT\06-Mar-2016\0\\#M062X/6-31+G(d,p) INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=671088640\\N_MMA_rad_AlCl3.MON.2.freq\\0,2\C,-8.2812558149,1.7294654654,1.5440902958\C,-7.5362646027,0.4727951018,1.1067187988\N,-6.1094267658,0.7638528042,0.9954074284\C,-5.9214262191,1.8657052179,0.0491352387\C,-6.7031478733,3.0843845645,0.5180274984\O,-8.081769867,2.7919836157,0.6388297378\H,-7.9341597356,2.0214407888,2.5479259356\H,-9.3567669476,1.5399576136,1.5781333977\H,-7.965060041,0.128762068,0.1466973878\H,-7.7085970626,-0.2991017035,1.8592056137\H,-6.270100413,1.5965488589,-0.9638468026\H,-4.8652217526,2.1298746364,-0.0213253538\H,-6.614947409,3.893746512,-0.2096096491\H,-6.3082188947,3.423950782,1.4882262103\C,-5.2112863268,-0.3822427789,0.8257851721\C,-5.5096117249,-1.4332662554,1.9015339487\C,-3.7599474485,0.0813188282,1.0027879357\H,-5.5374924019,-0.949114902,2.8824629188\H,-4.7185904344,-2.1886482471,1.9151776103\H,-6.4584370168,-1.9524069047,1.7426965664\H,-3.6758867055,0.6379942072,1.9405929046\H,-3.4129821448,0.7087192539,0.1791600709\H,-3.0912776617,-0.783415838,1.0521850554\C,-5.3923109493,-1.0164855842,-0.6214373519\H,-5.0827444351,-0.2570637841,-1.3467100925\H,-6.460174927,-1.2203531547,-0.7597523597\C,-4.6441888122,-2.2720402742,-0.8365056446\C,-3.3279601871,-2.2189886858,-1.3957475067\C,-5.2351439616,-3.6116578764,-0.5491985773\O,-2.7324931701,-1.1404383567,-1.6955189346\O,-2.7345421253,-3.3773695422,-1.5785612705\C,-1.4657723039,-3.3743134639,-2.2650502405\H,-4.583705369,-4.2099082559,0.0968104122\H,-5.3489002418,-4.176152486,-1.4832946017\H,-6.2141834011,-3.5127673498,-0.0805227145\H,-1.1093302849,-4.3993334835,-2.2031195288\H,-0.7777323986,-2.6812928663,-1.7799554744\H,-1.6189303323,-3.0785510418,-3.3053637004\Al,-2.6989537949,-0.1107743264,-3.2141162895\Cl,-0.6842512543,-0.1331693482,-3.8694381286\Cl,-4.0361767469,-1.2370822228,-4.4481185338\Cl,-3.4368700406,1.7918384139,-2.6294673826\\Version=ES64L-G09RevD.01\State=2-A\HF=-2373.7812992\S2=0.754177\S2-1=0.\S2A=0.750015\RMSD=1.963e-09\RMSF=1.588e-06\Dipole=-0.5975519,-2.5672503,2.4640505\Quadrupole=-2.0123,8.3040342,-6.2917341,-1.6543469,2.3089135,0.0811489\PG=C01 [X(C12H22Al1Cl3N1O3)]\\@

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