Supporting Information

Relative Reactivity of Various *Al*-substituted-dialkylalans in Reduction of Carbonyl Compounds; A Theoretical Study on Substituent Effect

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Received April 25, 2013, Accepted May 13, 2013

All geometries and energies of Alan(X), dimeric Alan(X)d and TS(X) were optimized at B3LYP/6-31+G(d). Frequency calculations have been carried out to determine all minima and transition states. Free energies are in hartree.

1. X = H

Alan(H), Free energy; -362.101948

Al	0.59233000	0.48146600	-0.00001000
C	2.39248600	-0.32389600	0.00000900
C	-1.04074700	-0.63788200	-0.00001400
H	0.46277900	2.07544300	-0.00000300
C	-2.39505700	0.09887200	0.00001400
H	2.97013400	0.00100000	-0.87789000
H	2.37815200	-1.42100800	-0.00022200
H	2.96994500	0.00062200	0.87817300
H	-0.98309000	-1.31466400	0.86934400
H	-0.98312000	-1.31465500	-0.86938000
H	-3.24555400	-0.59702800	0.00002600
H	-2.50480400	0.74433000	0.88072000
H	-2.50483500	0.74433500	-0.88068500

Alan(H)d, dimer, Free energy; -724.224817

Al	1.20622900	-0.53018900	-0.17043500
Al	-1.20625400	0.53011700	0.17029800
H	-0.19902200	-0.09854900	-1.12770800
H	0.19896000	0.09841300	1.12757400
C	-2.68423800	-0.73025800	0.55108000
C	-1.34439300	2.48901500	0.00988600
C	2.68414100	0.73024600	-0.55128300
C	1.34462300	-2.48902200	-0.00943900
C	3.88557500	0.64033000	0.41556300
C	-3.88570200	-0.64020800	-0.41571100
H	-2.29253800	-1.75793900	0.55865000
H	-1.73620700	2.93688900	0.93348200
H	-0.37656600	2.96193100	-0.19857100
H	2.29240500	1.75791200	-0.55894600
H	3.03223500	0.54511500	-1.57999400
H	0.37474500	-2.96322600	0.18615500
H	2.01942700	-2.77516100	0.80889000
H	4.32902400	-0.36390500	0.42284200
H	4.68559800	1.34228100	0.14238300
H	3.59456700	0.87275900	1.44841900
H	1.74906200	-2.93588600	-0.92806100
H	-2.02950300	2.77554300	-0.79968700
H	-3.59474000	-0.87249600	-1.44861300

H	-4.68572100	-1.34218700	-0.14259600
H	-4.32914200	0.36403000	-0.42282900
H	-3.03229100	-0.54521200	1.57981900

TS(H), Free energy; -555.183168

Al	1.39367900	-0.27216200	0.49897600
O	-0.17292900	-0.88708100	-0.18722200
C	-1.38840800	-0.37909900	-0.05608500
C	-2.04007600	-0.51860100	1.31778200
C	-2.30094400	-0.63006400	-1.24984300
H	1.39056500	-0.26446500	2.10398300
C	0.93150500	1.78111200	-0.10788700
C	2.96619200	-0.96248800	-0.47425100
C	-0.46159600	2.07097200	-0.18529500
H	-1.35057800	-0.21136300	2.10925100
H	-2.96012700	0.07211600	1.38684900
H	-2.29470300	-1.57408100	1.48360500
H	-1.78048000	-0.39627900	-2.18366000
H	-2.57699900	-1.69260100	-1.27437100
H	-3.22076500	-0.03853500	-1.18620200
H	1.45064100	2.21407100	0.75148000
H	1.48956800	1.85420600	-1.04243400
H	2.83603100	-0.92247700	-1.56440500
H	3.87331700	-0.39096400	-0.22975900
H	-1.17623500	0.90369800	-0.11620400
H	-0.88777400	2.35822100	-1.14893600
H	-0.94066000	2.56104800	0.66438800
H	3.17375500	-2.00884100	-0.20902600

2. X = F

Alan(F), Free energy; -461.448133

Al	-0.52226600	-0.03074200	0.00004300
C	-2.30435400	0.78581800	-0.00004200
C	1.20616900	0.91184300	0.00006200
F	-0.48092800	-1.71811600	0.00000800
C	2.47896300	0.04080800	-0.00006600
H	-2.88180300	0.47046500	-0.87997600
H	-2.26693200	1.88211600	0.00032600
H	-2.88227900	0.46985400	0.87935200
H	1.21409900	1.58932300	0.86991900
H	1.21404000	1.58946100	-0.86969100
H	3.39046300	0.65371000	-0.00009500
H	2.52283900	-0.61156100	0.88004300
H	2.52271800	-0.61148800	-0.88023300

Alan(F)d (dimer), Free energy; -922.934723

Al	0.84840929	1.07452861	-0.49018552
C	1.38225354	1.00753246	-2.38284683
C	1.31607354	2.44899952	0.82504231
F	1.00695746	-0.61815207	0.28113711
F	-0.95011584	0.61022712	-0.32894012
Al	-0.79156826	-1.08244367	0.44240428
C	-1.25927001	-2.45693210	-0.87279144
C	-1.32537504	-1.01541276	2.33507485
C	-2.84948833	-1.04460024	2.59271842
C	2.90636766	1.03692362	-2.64046111
H	0.94870138	0.11103974	-2.85134948
H	0.91257833	1.85819041	-2.90249524

H	0.85218947	2.27030234	1.80378321
H	0.99939964	3.44703384	0.49173620
H	2.40202658	2.49919991	0.98506429
H	-2.34521397	-2.50700699	-1.03291569
H	-0.94275150	-3.45498634	-0.53939824
H	-0.79527032	-2.27834651	-1.85149791
H	-0.89169060	-0.11899108	2.80359070
H	-0.85580784	-1.86614827	2.85469425
H	-3.31649283	-1.94666029	2.17631215
H	-3.08440577	-1.02805711	3.66563829
H	-3.35472257	-0.18081067	2.14112187
H	3.14130852	1.02038942	-3.71337599
H	3.37323972	1.93905667	-2.22406475
H	3.41171212	0.17321325	-2.18883617

TS(F), Free energy; -654.531707

Al	1.26575900	-0.21169400	0.00742800
O	-0.34348400	-0.77261000	-0.57563800
C	-1.53591100	-0.36328500	-0.15009000
C	0.71404700	1.87628000	-0.06840600
C	-0.67156800	2.09666300	0.17071700
H	-1.35500600	0.88864400	0.07655300
F	1.41607900	-0.49263100	1.68474600
C	2.78496800	-0.71475200	-1.12642600
C	-1.97131600	-0.87811500	1.21927000
C	-2.60878800	-0.36156200	-1.23167200
H	1.09300300	2.19683900	-1.04000100
H	1.37263300	2.12443700	0.76929400
H	-1.27692100	2.56939900	-0.60507900
H	-0.99724500	2.32903800	1.18571000
H	2.58850800	-0.52635700	-2.19010700
H	3.01858400	-1.78296500	-1.02085800
H	3.69489800	-0.16256600	-0.85478500
H	-1.17121100	-0.75020500	1.95424300
H	-2.18884700	-1.95162900	1.14071700
H	-2.87672800	-0.36868900	1.56731200
H	-2.86607000	-1.39869200	-1.48344100
H	-2.23659400	0.12260200	-2.13989100
H	-3.51929700	0.14535800	-0.89419400

3. X = Cl

Alan(Cl), Free energy; -821.793634

Al	0.36888000	-0.43041000	-0.00893700
C	1.91371700	-1.63643700	0.02927500
C	-1.52082600	-0.98166000	-0.05620600
C	-2.59809600	0.11515400	0.04871200
Cl	0.80459700	1.66484400	-0.00700700
H	2.58734300	-1.44112300	-0.81596000
H	1.62211800	-2.69336500	-0.00849800
H	2.50746100	-1.48443600	0.94107800
H	-1.65937100	-1.72640100	0.74482800
H	-1.66071500	-1.55627700	-0.98731400
H	-3.61067300	-0.30700900	-0.00272200
H	-2.52164100	0.66858500	0.99209700
H	-2.50688700	0.85065800	-0.75889200

Alan(Cl)d, dimer, Free energy; -1643.59878

Al	1.55938400	-0.59482400	-0.11993300

C	2.91343900	0.66770300	-0.78920000
C	1.80985600	-2.45902800	0.42969100
Cl	-0.30182200	-0.48965800	-1.55516800
Cl	0.30181500	0.48965100	1.55517800
Al	-1.55938700	0.59482900	0.11993900
C	-1.80984000	2.45903900	-0.42967400
C	-2.91345400	-0.66769100	0.78919300
C	4.10110100	0.91788600	0.16623600
C	-4.10108500	-0.91790300	-0.16627300
H	2.42769300	1.62306300	-1.03498900
H	3.29075600	0.27797800	-1.74818700
H	0.87377300	-2.92056900	0.76738200
H	2.53151200	-2.53773900	1.25427400
H	2.19723300	-3.06746900	-0.39911700
H	-2.19703900	3.06751500	0.39919100
H	-2.53163300	2.53778200	-1.25413500
H	-0.87378700	2.92051800	-0.76753200
H	-3.29080400	-0.27794800	1.74816000
H	-2.42771000	-1.62304300	1.03501800
H	4.63936300	-0.00958700	0.40099100
H	4.83318300	1.61270000	-0.26720800
H	3.77134200	1.35278400	1.11852400
H	-4.83317400	-1.61271500	0.26716200
H	-4.63935000	0.00956000	-0.40106200
H	-3.77129400	-1.35281600	-1.11854300

TS(Cl), Free energy; -1014.876707

Al	-1.05137400	-0.38887600	-0.24964300
O	0.60122500	-0.26878000	-0.93745900
C	1.73149400	0.15333000	-0.37111300
C	-0.35385200	-1.11001600	1.66486700
C	0.95505900	-0.66816600	2.00196600
H	1.57328800	-0.13990400	0.85941000
Cl	-1.88014300	1.58287000	0.18184300
C	-2.25117100	-1.62397200	-1.18717200
C	1.93779600	1.66515700	-0.33110000
C	2.95487400	-0.66585700	-0.76582400
H	-0.48402700	-2.18859400	1.56087400
H	-1.16250800	-0.61592300	2.21041600
H	1.74628000	-1.40450600	2.15311100
H	1.06453000	0.23119800	2.60926000
H	-1.78023600	-2.59848900	-1.37242000
H	-2.55226800	-1.21272400	-2.15992700
H	-3.17311700	-1.80043300	-0.61724400
H	1.05099200	2.17317200	0.05735200
H	2.11129400	2.02420400	-1.35412600
H	2.80848400	1.93067800	0.27860400
H	3.19769300	-0.46299700	-1.81685000
H	2.74831500	-1.73629000	-0.66874400
H	3.82658300	-0.40541900	-0.15575600

4. X = OMe

Alan(OMe), Free energy; -476.666373

Al	0.07352800	0.48943600	-0.00417800
C	1.18832100	2.11590800	0.00579200
C	-1.89716400	0.48403900	-0.00962900
C	-2.59505800	-0.89061200	0.00964700
O	0.83953900	-1.05264600	-0.00344200

C	2.91343900	0.66770300	-0.78920000
C	1.80985600	-2.45902800	0.42969100
Cl	-0.30182200	-0.48965800	-1.55516800
Cl	0.30181500	0.48965100	1.55517800
Al	-1.55938700	0.59482900	0.11993900
C	-1.80984000	2.45903900	-0.42967400
C	-2.91345400	-0.66769100	0.78919300
C	4.10110100	0.91788600	0.16623600
C	-4.10108500	-0.91790300	-0.16627300
H	2.42769300	1.62306300	-1.03498900
H	3.29075600	0.27797800	-1.74818700
H	0.87377300	-2.92056900	0.76738200
H	2.53151200	-2.53773900	1.25427400
H	2.19723300	-3.06746900	-0.39911700
H	-2.19703900	3.06751500	0.39919100
H	-2.53163300	2.53778200	-1.25413500
H	-0.87378700	2.92051800	-0.76753200
H	-3.29080400	-0.27794800	1.74816000
H	-2.42771000	-1.62304300	1.03501800
H	4.63936300	-0.00958700	0.40099100
H	4.83318300	1.61270000	-0.26720800
H	3.77134200	1.35278400	1.11852400
H	-4.83317400	-1.61271500	0.26716200
H	-4.63935000	0.00956000	-0.40106200
H	-3.77129400	-1.35281600	-1.11854300

TS(Cl), Free energy; -1014.876707

Al	-1.05137400	-0.38887600	-0.24964300
O	0.60122500	-0.26878000	-0.93745900
C	1.73149400	0.15333000	-0.37111300
C	-0.35385200	-1.11001600	1.66486700
C	0.95505900	-0.66816600	2.00196600
H	1.57328800	-0.13990400	0.85941000
Cl	-1.88014300	1.58287000	0.18184300
C	-2.25117100	-1.62397200	-1.18717200
C	1.93779600	1.66515700	-0.33110000
C	2.95487400	-0.66585700	-0.76582400
H	-0.48402700	-2.18859400	1.56087400
H	-1.16250800	-0.61592300	2.21041600
H	1.74628000	-1.40450600	2.15311100
H	1.06453000	0.23119800	2.60926000
H	-1.78023600	-2.59848900	-1.37242000
H	-2.55226800	-1.21272400	-2.15992700
H	-3.17311700	-1.80043300	-0.61724400
H	1.05099200	2.17317200	0.05735200
H	2.11129400	2.02420400	-1.35412600
H	2.80848400	1.93067800	0.27860400
H	3.19769300	-0.46299700	-1.81685000
H	2.74831500	-1.73629000	-0.66874400
H	3.82658300	-0.40541900	-0.15575600

4. X = OMe

Alan(OMe), Free energy; -476.666373

Al	0.07352800	0.48943600	-0.00417800
C	1.18832100	2.11590800	0.00579200
C	-1.89716400	0.48403900	-0.00962900
C	-2.59505800	-0.89061200	0.00964700
O	0.83953900	-1.05264600	-0.00344200

C	2.17474300	-1.50267300	0.00052800
H	1.75337200	2.21054200	0.94419800
H	0.58688900	3.02744600	-0.10392700
H	1.92933400	2.11022600	-0.80562400
H	-2.22904200	1.05965000	-0.88981200
H	-2.23442600	1.08760100	0.84945700
H	-3.68964900	-0.79334200	0.00234800
H	-2.31286200	-1.49825300	-0.85821000
H	-2.32235500	-1.46888900	0.90038300
H	2.35854700	-2.11884600	0.89118500
H	2.36232100	-2.12285700	-0.88654300
H	2.90063500	-0.67475400	0.00037200

Alan(OMe)d, dimer, Free energy; -953.387007

Al	1.35546000	-0.42974300	-0.26052200
C	2.78054900	-0.03185800	1.06150500
C	1.76525700	-1.43121300	-1.91328900
O	0.21563000	1.03554600	-0.58362700
C	0.52154900	2.31968900	-1.12381600
O	-0.21563000	-1.03552200	0.58364700
Al	-1.35545500	0.42977400	0.26055300
C	-0.52161400	-2.31975000	1.12359800
C	-2.78057900	0.03192000	-1.06144700
C	-1.76520500	1.43124500	1.91333100
C	4.11726600	0.48590300	0.48538500
C	-4.11722900	-0.48599300	-0.48530700
H	2.39954200	0.68346200	1.80748700
H	2.97882400	-0.95405900	1.63418600
H	0.87354200	-1.61064600	-2.52946500
H	2.21253500	-2.41269900	-1.69650900
H	2.49135200	-0.89901800	-2.54539200
H	-0.40344000	2.83566700	-1.40206000
H	1.13870000	2.20773900	-2.02213200
H	1.06033000	2.92649300	-0.38658800
H	-1.13875700	-2.20793200	2.02193700
H	0.40335000	-2.83582500	1.40174600
H	-1.06042700	-2.92639400	0.38626200
H	-2.39956800	-0.68329300	-1.80753100
H	-2.97895200	0.95417100	-1.63401300
H	-2.49128500	0.89905700	2.54545700
H	-2.21247600	2.41273700	1.69656600
H	-0.87346600	1.61066400	2.52947600
H	3.99247200	1.44347800	-0.03908300
H	4.87537400	0.64832200	1.26483400
H	4.54651900	-0.21944600	-0.23829000
H	-4.87537100	-0.64837200	-1.26473100
H	-3.99234500	-1.44361900	0.03904400
H	-4.54648600	0.21924800	0.23847200

TS(OMe), Free energy; -669.745327

Al	-0.94135000	-0.46644900	-0.23501800
O	0.67408000	-0.11089200	-0.97128700
C	1.74081000	0.39016900	-0.35958600
C	-0.04472500	-1.50924100	1.43776600
C	1.21990600	-0.97799600	1.81835200
H	1.70109200	-0.16902500	0.80295800
O	-1.63000100	0.93742900	0.54702800
C	-2.08193400	-1.58883500	-1.38358100
C	1.67571800	1.87245500	-0.00068400

C	3.06744300	-0.10173000	-0.92480100
C	-2.77034400	1.71637800	0.28931000
H	-0.05476000	-2.55338000	1.12169600
H	-0.87779600	-1.23008100	2.08848700
H	2.09750000	-1.62758700	1.80186800
H	1.25070900	-0.21732900	2.59988700
H	-1.51966900	-2.42528200	-1.82010900
H	-2.50697900	-1.01675400	-2.22030200
H	-2.92845300	-2.01730800	-0.82889600
H	0.72524800	2.10430600	0.48898400
H	1.73718500	2.46353400	-0.92448800
H	2.50881400	2.16385100	0.64885900
H	3.22550100	0.34614200	-1.91475500
H	3.05149600	-1.18935700	-1.04628900
H	3.90839900	0.18166100	-0.28242000
H	-3.26302000	1.98584200	1.23520400
H	-3.51141700	1.19275900	-0.33639600
H	-2.50017600	2.65235600	-0.22562700

5. X = NMe_2

Alan(NMe_2), Free energy; -496.048975

Al	0.25978000	0.31664300	-0.00006400
C	0.57108500	2.26683200	0.00000800
C	1.69754000	-1.05164400	-0.00002800
C	3.14290000	-0.51057800	0.00004700
N	-1.44913200	-0.26591600	-0.00009200
C	-1.83305900	-1.67075700	0.00004400
C	-2.61182200	0.61081400	0.00003600
H	0.12847100	2.75330900	-0.88045100
H	1.64203500	2.50641800	-0.00121300
H	0.13067800	2.75266300	0.88194700
H	1.55335300	-1.70977300	-0.87181300
H	1.55329900	-1.70980800	0.87172000
H	3.88638700	-1.31973800	-0.00003400
H	3.34490100	0.11156500	-0.88149100
H	3.34488100	0.11137900	0.88173100
H	-2.43592500	-1.92652600	0.88848200
H	-2.43639500	-1.92654300	-0.88806600
H	-0.94867300	-2.31689300	-0.00017700
H	-3.24492500	0.44435600	0.88859800
H	-2.30596600	1.66243900	-0.00010600
H	-3.24520400	0.44420100	-0.88829600

Alan(NMe_2)d, dimer, Free energy; -992.128223

Al	1.32260600	-0.37889100	-0.41190100
N	-0.30208800	-1.34439800	0.26762800
N	0.30216600	1.34447700	-0.26715300
C	2.81593700	-0.50314200	0.90548200
C	1.71319700	-0.83254500	-2.30526800
C	0.87103700	2.31914000	0.69491800
Al	-1.32271300	0.37890500	0.41185600
C	-0.87091000	-2.31953000	-0.69399800
C	-2.81549800	0.50292600	-0.90616500
C	-1.71418400	0.83262200	2.30502500
C	4.12599500	0.20355600	0.49095600
C	-4.12571000	-0.20373700	-0.49206600
C	0.09461300	2.03507200	-1.56316300
C	-0.09433300	-2.03445500	1.56389600

H	2.51269100	-0.13982000	1.90037100
H	3.03098100	-1.57493000	1.05519000
H	0.84928200	-0.80192700	-2.98296000
H	2.13915100	-1.84403800	-2.38348100
H	2.46706300	-0.15066000	-2.72570000
H	0.18201400	3.16042200	0.85647000
H	1.82105100	2.72841600	0.32315100
H	1.05958500	1.84488500	1.66026400
H	-1.82086000	-2.72875100	-0.32200700
H	-0.18180700	-3.16081200	-0.85522100
H	-1.05954200	-1.84570900	-1.65953900
H	-2.51183400	0.13945000	-1.90087200
H	-3.03050400	1.57468400	-1.05613100
H	-2.46806000	0.15058000	2.72518500
H	-2.14041700	1.84401400	2.38300100
H	-0.85054700	0.80225000	2.98307900
H	3.99146900	1.28940000	0.39232900
H	4.93471000	0.04969300	1.21988900
H	4.49365400	-0.16120700	-0.47711600
H	-4.93411800	-0.05003800	-1.22137400
H	-3.99119100	-1.28955700	-0.39317200
H	-4.49379200	0.16120000	0.47577800
H	-0.59021600	2.88722000	-1.44826500
H	1.04580900	2.41595500	-1.96110400
H	-0.33273300	1.35266800	-2.30078200
H	-1.04544800	-2.41528200	1.96207900
H	0.59058800	-2.88656400	1.44926900
H	0.33300400	-1.35172300	2.30121900

TS(NMe_2), Free energy; -689.117721

Al	0.70101400	-0.65182100	0.39318800
O	-0.91454700	-0.02091000	0.92115500
C	-1.92364900	0.46508800	0.21518700
C	-0.10976500	-1.59226200	-1.39464300
C	-1.33516200	-1.02746800	-1.85653900
H	-1.82954900	-0.17697100	-0.91221500
N	1.79274200	0.72582100	-0.15921200
C	1.38026200	-2.04908000	1.61544700
C	-1.80131800	1.91405300	-0.24756700
C	-3.29805400	0.04618700	0.72253700
C	2.94135300	0.52227200	-1.02177300
C	1.89359600	1.98421400	0.55891800
H	-0.15328300	-2.63684700	-1.08277100
H	0.76497000	-1.35142100	-2.00486200
H	-2.22941900	-1.65429700	-1.87668100
H	-1.29950100	-0.29664800	-2.66651900
H	0.61781200	-2.80160100	1.86040300
H	1.72410300	-1.61292400	2.56429900
H	2.24139400	-2.58289800	1.18763400
H	-0.82381900	2.09095900	-0.70427500
H	-1.89889500	2.57700100	0.62274700
H	-2.59070500	2.17172700	-0.96243000
H	-3.50468100	0.56316400	1.66909300
H	-3.32124300	-1.03064500	0.91612800
H	-4.08829100	0.30696500	0.01010500
H	2.87044100	-0.43164100	-1.56171500
H	3.89933100	0.50802700	-0.46581900
H	3.02739500	1.31967500	-1.78347600
H	2.80872100	2.04734700	1.17992800

H	1.03506000	2.12436000	1.22618900
H	1.92057500	2.84884100	-0.13137300

6. X = OAc

Alan(OAc), Free energy; -590.053034

Al	-0.67988300	0.60909200	-0.00023100
C	-1.00715800	2.54561200	-0.00050100
O	0.86542100	0.10740200	-1.08712700
C	-2.08248800	-0.77775200	0.00026500
C	-1.61077800	-2.24681200	-0.00027200
C	1.50848400	-0.10621600	0.00084500
C	2.92086100	-0.60408000	0.00002800
O	0.86516400	0.10804000	1.08828800
H	-1.58669700	2.85583000	-0.88131200
H	-0.07553200	3.12639100	-0.00235000
H	-2.73295000	-0.60135400	0.87253700
H	-2.73396000	-0.60103300	-0.87118500
H	-1.00009800	-2.47451600	0.88292700
H	3.43243300	-0.30153800	0.91613000
H	3.45113700	-0.23969700	-0.88275300
H	2.90436600	-1.70037000	-0.04037600
H	-1.58361400	2.85654200	0.88208300
H	-2.45347700	-2.95225300	0.00021600
H	-1.00133200	-2.47424500	-0.88439100

Alan(OAc)d, dimer, Free energy; -1180.127122

Al	-1.95066200	-0.43623200	0.38870700
C	-3.73427100	-0.74933700	-0.39688900
C	-1.54271800	-0.53708300	2.31752000
O	0.76361000	1.71322200	-0.33284500
O	-0.82659600	-1.64353600	-0.49656800
C	-0.45273100	2.05984400	-0.33855700
Al	2.14888500	0.46569800	-0.26036400
C	0.37655400	-1.97207600	-0.72584800
C	3.27059200	0.84311100	-1.83490700
C	2.80422800	0.44192700	1.60569000
C	0.64125200	-3.39394800	-1.15258300
O	1.36762800	-1.19576600	-0.60548600
C	-0.76764100	3.52705000	-0.48657500
O	-1.42846400	1.26042600	-0.21102400
C	-4.86600200	0.17365600	0.10383100
C	3.94516100	-0.55719200	1.89748300
H	-4.01623500	-1.79864200	-0.21146100
H	-3.65601900	-0.66612000	-1.49310300
H	-0.48883000	-0.32630800	2.54675300
H	-1.76514700	-1.53489500	2.72251400
H	-2.14475100	0.17803000	2.89620300
H	4.09090500	0.11882400	-1.93702500
H	3.73036400	1.83984800	-1.77606800
H	2.69552000	0.80978400	-2.77123300
H	1.96292600	0.24095200	2.28772700
H	3.14280800	1.45885800	1.86304000
H	1.57707100	-3.46435700	-1.71015300
H	0.72877100	-4.01363800	-0.25084000
H	-0.19540000	-3.77726200	-1.74108100
H	-1.72419400	3.66319800	-0.99582900
H	0.03503000	4.04465400	-1.01539300

H	-0.85529400	3.96266700	0.51716200
H	-5.83251600	-0.05357600	-0.36863200
H	-5.01232500	0.08420900	1.18873400
H	-4.64832200	1.22983200	-0.10444800
H	4.27741300	-0.51761200	2.94470300
H	3.63806600	-1.59274200	1.69829800
H	4.82728600	-0.35925300	1.27404800

TS(OAc), Free energy; -783.117464

Al	0.21324000	1.21165400	-0.15211100
O	-1.14487500	0.31451300	-0.89700500
C	-1.90299600	-0.68923500	-0.45679800
C	-0.38285400	0.85639400	1.87070800
C	-1.21535800	-0.28714000	2.04083700
H	-1.69807000	-0.69536600	0.79838300
O	1.82169300	0.42108600	-0.41663700
C	0.33190200	3.10579000	-0.65193100
C	-1.45662200	-2.08602400	-0.87420500
C	-3.40029800	-0.41628400	-0.55681200
C	2.21554000	-0.76757100	0.00500500
C	3.62654100	-1.12713200	-0.41389400
O	1.51161100	-1.51961800	0.67761300
H	-0.81669100	1.81194100	2.17265700
H	0.64605100	0.70940200	2.21308100
H	-2.21659100	-0.16330300	2.45789900
H	-0.73733400	-1.23902700	2.26964600
H	-0.62650700	3.62838500	-0.53270800
H	0.63676800	3.21921200	-1.70136200
H	1.07708700	3.64023400	-0.04667300
H	-0.40263300	-2.23826300	-0.62994600
H	-1.58947300	-2.18824400	-1.95961900
H	-2.05708100	-2.85812400	-0.38042100
H	-3.69347600	-0.41739400	-1.61458500
H	-3.64058800	0.56778500	-0.14193000
H	-3.98462100	-1.18362800	-0.03746900
H	4.32858700	-0.37063800	-0.04558800
H	3.69916800	-1.12545500	-1.50750400
H	3.90072400	-2.10964600	-0.02563500

7. X = OMs

Alan(OMs), Free energy; -1025.286898

Al	1.01774200	0.73206500	0.00003000
C	1.02929100	2.69743400	-0.00010400
O	-0.40109600	0.04454800	1.17535300
C	2.62705700	-0.39847000	0.00022300
C	2.41200900	-1.92648200	-0.00021500
S	-1.28998400	-0.41090600	0.00002400
C	-2.74100200	0.64628500	-0.00011600
O	-0.40100300	0.04436400	-1.17530400
O	-1.71996400	-1.79936900	0.00011600
H	-3.31731900	0.41285200	-0.89801200
H	-2.41519000	1.68737100	-0.00018900
H	-3.31738500	0.41299900	0.89777600
H	1.55478400	3.09122200	-0.88144600
H	1.55486400	3.09132800	0.88114300
H	3.23810000	-0.11134100	-0.87138400
H	3.23753600	-0.11176900	0.87236700
H	1.84877200	-2.25514000	-0.88222300

H	1.84813700	-2.25556200	0.88123100
H	3.36470300	-2.47377900	-0.00000100
H	0.02447200	3.14052400	-0.00008300

Alan(OMs)d, dimer, Free energy; -2050.568058

Al	2.09462700	0.75151900	0.24237600
C	3.68039300	1.09403400	-0.87559700
C	2.02470600	0.87573000	2.20742800
O	-0.74703700	-1.86771100	0.48887700
O	0.74702000	1.86769600	-0.48889000
S	0.73536400	-2.15163300	0.27232600
Al	-2.09462800	-0.75152400	-0.24240700
S	-0.73537300	2.15163100	-0.27229800
C	-2.02466300	-0.87571800	-2.20745800
C	-3.68041700	-1.09405300	0.87552800
C	-0.80947300	3.35140800	1.05773700
O	-1.39727000	0.91616600	0.33564700
C	0.80950600	-3.35145200	-1.05766800
O	1.39725600	-0.91617900	-0.33564400
O	-1.38904200	2.68038800	-1.46082300
O	1.38901500	-2.68034300	1.46088200
C	-4.91267400	-0.21422200	0.57251400
C	4.91268600	0.21426900	-0.57253800
H	3.39531800	0.97666500	-1.93257900
H	3.95857600	2.15511300	-0.77134700
H	1.03467200	0.65036100	2.62786400
H	2.31345500	1.87742300	2.55875100
H	2.72434000	0.16738700	2.67168400
H	-2.72428100	-0.16736800	-2.67172600
H	-2.31341100	-1.87740700	-2.55879500
H	-1.03461700	-0.65035500	-2.62787000
H	-3.39534900	-0.97676300	1.93252000
H	-3.95864000	-2.15511400	0.77120600
H	-1.86310700	3.55167300	1.26208300
H	-0.31081200	2.93533500	1.93465700
H	-0.30504400	4.25456900	0.70818100
H	1.86314600	-3.55171600	-1.26198200
H	0.31086400	-2.93541100	-1.93461300
H	0.30507600	-4.25460600	-0.70809600
H	-5.76284300	-0.45047500	1.22785400
H	-4.69243100	0.85335900	0.70675900
H	-5.26012000	-0.34157100	-0.46124600
H	4.69248200	-0.85332800	-0.70671200
H	5.76283900	0.45051200	-1.22790300
H	5.26013700	0.34169900	0.46121000

TS(OMs), Free energy; -1218.358763

Al	-0.40955400	1.30626700	-0.24121100
O	-1.70328800	0.25817400	-0.87319700
C	-2.32545700	-0.81305400	-0.36929800
C	-0.75470100	0.87664300	1.82315300
C	-1.41500400	-0.36172000	2.05579500
H	-1.98300300	-0.82189800	0.84271400
O	1.24275300	0.63737000	-0.63415000
C	-0.49328600	3.18838200	-0.77489100
C	-1.82247100	-2.15900100	-0.87904300
C	-3.84154700	-0.65886700	-0.29889500
S	2.11894100	-0.45775700	0.07607200
C	3.49973500	-0.57981900	-1.06833400

O	2.61641700	0.05427100	1.36309600
O	1.40562500	-1.74881400	0.09160600
H	-1.28709800	1.76787600	2.16306600
H	0.31038800	0.87342700	2.07925300
H	-2.38126700	-0.37316200	2.56266400
H	-0.80679600	-1.25243800	2.21617300
H	-1.48483100	3.62470000	-0.59644800
H	-0.27385500	3.30515600	-1.84488600
H	0.24107600	3.79623300	-0.22972200
H	-0.73651000	-2.23021600	-0.77911800
H	-2.08618900	-2.25174100	-1.94108500
H	-2.29186000	-2.98666200	-0.33563700
H	-4.24762200	-0.65567900	-1.31849800
H	-4.11188400	0.29108900	0.17352800
H	-4.30395800	-1.48446300	0.25289300
H	3.98453800	0.39592900	-1.13001400
H	3.11840500	-0.89182800	-2.04212400
H	4.18594200	-1.32706800	-0.66393100