Electronic Suplementary Information to Insights into the Structure and Stability of the Carbonic Acid Dimer

Juliana Murillo, Jorge David, Albeiro Restrepo.

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1 Cartesian coordinates of all MP2/6-311++G** optimized dimers

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Structure 1,Ia:aa+aa
C -1.89055100 -0.01943100 0.00000400
O -1.22046100 -1.04749300 0.00016200
O -3.22568400 -0.02670600 -0.00006000
H -3.48378200 -0.95718900 0.00002100
O -1.43937900 1.21103500 -0.00012100
H -0.45022800 1.16939600 -0.00002300
C 1.89055100 0.01943100 0.00001300
O 1.22046200 1.04749300 0.00018900
O 3.22568400 0.02670500 -0.00007800
H 3.48378200 0.95718800 -0.00000700
O 1.43937800 -1.21103500 -0.00010500
H 0.45022800 -1.16939600 0.00000800

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Structure 2,Ib:aa+as
C 1.88588000 -0.03350800 -0.00002400
O 1.19828200 -1.05145400 -0.00028800

O 1.45791200 1.20344000 0.00012900
H 0.46724900 1.18439000 -0.00001400
O 3.22030200 -0.06696800 0.00013100
H 3.46054500 -1.00216800 0.00001800
C -1.88570700 0.08752900 -0.00000700
O -1.19924700 1.09237200 -0.00020300
O -3.21875000 0.16012000 0.00004700
H -3.56030300 -0.74280000 0.00017500
O -1.44764800 -1.16483100 0.00018000
H -0.45534600 -1.14498000 0.00003800

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Structure 3,Ic:as+as
C 1.87944800 0.10132100 -0.00001400
O 1.17634000 1.09608100 -0.00013200
O 3.21047700 0.19972200 0.00006000
H 3.56920300 -0.69662300 0.00013100
O 1.46458500 -1.15685500 0.00005400
H 0.47106500 -1.15946900 -0.00001700
C -1.87944200 -0.10132100 -0.00000600
O -1.17632000 -1.09607500 -0.00011000
O -3.21046800 -0.19974600 0.00004300
H -3.56920400 0.69659500 0.00010800
O -1.46461400 1.15687000 0.00007300
H -0.47110000 1.15951200 -0.00000200

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Structure 4,Id:aa+as
C 1.91015100 -0.02963100 -0.00101500
O 1.20956400 -1.00484200 0.22699400
O 3.23961100 -0.07141300 -0.07939400
H 3.48519400 -0.99493300 0.06144000
O 1.48437800 1.20415400 -0.20076200
H 0.51372600 1.18244300 -0.08999200
C -2.10876100 -0.07448300 -0.01507100
O -3.28709500 0.09685200 -0.15483800
O -1.46665000 -1.21972700 -0.11872700
H -0.50435600 -1.10665600 0.04537900
O -1.24210000 0.96884200 0.29267000
H -1.80456900 1.75290800 0.35214000

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Structure 5,Ie:as+as
C -2.10764300 -0.05705400 -0.01682000
O -3.28183100 0.13981900 -0.15775300

O -1.48836100 -1.21301100 -0.12334300
H -0.52417500 -1.12332200 0.04599000
O -1.22219100 0.97163700 0.29611800
H -1.77395500 1.76278100 0.36177700
C 1.90623000 -0.09595300 0.00881400
O 1.18869400 -1.04832200 0.22755800
O 3.23275700 -0.20424500 -0.05142200
H 3.59727800 0.67397800 -0.21835100
O 1.49433100 1.15962800 -0.19788100
H 0.52213900 1.16055400 -0.08759700

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Structure 6,IIa:aa+aa
C -2.08590100 0.03110400 -0.00817300
O -1.45929600 1.04207500 0.25790700
O -3.40286400 -0.00188500 -0.22874400
H -3.70701000 0.90968100 -0.13383600
O -1.59285500 -1.19567600 -0.12539600
H -0.63691500 -1.13805400 0.04722800
C 2.17842200 0.13527500 -0.00220000
O 2.57951900 1.21583300 -0.35451100
O 2.87403200 -1.01301700 -0.02291600
H 3.74550700 -0.78384100 -0.36952000
O 0.95479700 -0.13106400 0.48273300
H 0.41662800 0.68380300 0.44578400

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Structure 7,IIIa:aa+as
C 1.68234300 -0.11356900 -0.08148500
O 0.85414000 -0.97550400 -0.30440300
O 2.99470500 -0.35250100 0.08487900
H 3.09326400 -1.30742500 -0.01228100
O 1.46344000 1.18772500 0.03638800
H 0.50354000 1.32911900 -0.08507600
C -1.69844400 0.17169800 0.03607700
O -1.26382800 1.18986200 -0.45146000
O -1.57394300 -0.12957000 1.32571600
H -1.85945100 -1.04317900 1.45105800
O -2.38545500 -0.77036200 -0.63075600
H -2.35322400 -0.52449000 -1.56415600

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Structure 8,IIIb:aa+as
C -1.68229600 -0.11358300 -0.08176700
O -0.85450400 -0.97564600 -0.30552400

O -1.46299800 1.18762000 0.03619100
H -0.50320500 1.32884800 -0.08601100
O -2.99458300 -0.35222600 0.08561700
H -3.09343700 -1.30710900 -0.01163100
C 1.69840100 0.17166500 0.03613000
O 1.26416400 1.18942100 -0.45265800
O 1.57282000 -0.12853300 1.32588100
H 1.85852700 -1.04196600 1.45242500
O 2.38596800 -0.77093900 -0.62926500
H 2.35454700 -0.52583900 -1.56289200

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Structure 9,IIb:aa+as
C -2.06646800 0.04239400 -0.01094300
O -1.39245900 1.02916200 0.23304900
O -3.38605700 0.06738400 -0.21616600
H -3.64733800 0.99279200 -0.12834900
O -1.63157900 -1.20594100 -0.11591300
H -0.67128700 -1.19268600 0.04435500
C 2.20192600 -0.10062900 0.02124300
O 2.98217000 -1.00021200 -0.12322200
O 0.94889100 -0.25810700 0.47570800
H 0.44912000 0.58109600 0.44942100
O 2.44204900 1.20685500 -0.23746700
H 3.35263400 1.25508000 -0.55513700

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Structure 10,IIIc:as+as
C -1.66492000 -0.18318100 -0.09434900
O -0.82114200 -1.01638100 -0.31469900
O -2.96267100 -0.48883600 0.07241100
H -3.43606700 0.33519400 0.23855300
O -1.46833000 1.14063500 0.01826300
H -0.51144500 1.30886100 -0.10275800
C 1.69058800 0.18822400 0.03992300
O 1.24473800 1.19742600 -0.45836400
O 1.55787200 -0.10457700 1.33022300
H 1.84164800 -1.01788700 1.46366400
O 2.39818000 -0.74600900 -0.61317800
H 2.36267900 -0.51449700 -1.55015400

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Structure 11,IIId:as+as
C 1.66498700 -0.18317500 -0.09438300
O 0.82129200 -1.01644200 -0.31480200

O 2.96276000 -0.48872100 0.07239200
H 3.43607800 0.33534200 0.23858500
O 1.46827800 1.14061600 0.01830000
H 0.51138600 1.30879600 -0.10272800
C -1.69065000 0.18821700 0.03996200
O -1.24484700 1.19750300 -0.45819700
O -1.55782700 -0.10479100 1.33020400
H -1.84156100 -1.01813300 1.46351200
O -2.39829200 -0.74591300 -0.61323000
H -2.36284000 -0.51427100 -1.55017600

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Structure 12,IIc:aa+as
C -2.18701100 0.11824000 -0.00318700
O -2.63437500 1.18235700 -0.34771700
O -0.94564000 -0.10256100 0.46093600
H -0.43646100 0.73009400 0.41506400
O -2.83801900 -1.05649400 -0.01272000
H -3.72377700 -0.86108900 -0.34352400
C 2.09216900 0.10038200 -0.00265900
O 1.45674900 1.10264400 0.22696300
O 3.41382500 0.11026400 -0.19516600
H 3.69773100 -0.79815900 -0.35561800
O 1.59676300 -1.14709800 -0.09969700
H 0.63712800 -1.09548200 0.05837000

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Structure 13,IId:as+as
C -2.19961200 -0.11822200 0.02005100
O -2.94748700 -1.04577400 -0.11962900
O -0.93961700 -0.23230700 0.47035500
H -0.46504000 0.62110900 0.43595000
O -2.48497800 1.17873200 -0.23885000
H -3.39765100 1.19670400 -0.55374200
C 2.06753800 0.11107300 -0.00539500
O 1.38597300 1.08649700 0.21155800
O 3.38732100 0.18254600 -0.19685400
H 3.71445900 -0.71300500 -0.34751300
O 1.63258300 -1.15828200 -0.08771300
H 0.67032300 -1.15321900 0.06642900

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Structure 14,IIIe:aa+aa
C 1.71339900 -0.10671400 -0.11324500
O 0.92615800 -0.94733500 -0.49400500

O 1.44136000 1.16948500 0.14714800
H 0.48811900 1.27999300 -0.00856900
O 3.01949000 -0.32468100 0.11222400
H 3.16291900 -1.25587700 -0.09684200
C -1.84362600 -0.03695700 0.03568900
O -2.52859000 -0.82062100 -0.56488100
O -1.36724700 1.13214300 -0.46186000
H -1.66342200 1.16703500 -1.38111300
O -1.42841800 -0.12563900 1.30358700
H -1.70827500 -0.99594000 1.61414400

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Structure 15,IIIf:aa+aa
C 1.84355500 -0.03701800 0.03593900
O 2.52855400 -0.82009500 -0.56528800
O 1.42812800 -0.12683400 1.30369400
H 1.70814700 -0.99733200 1.61355400
O 1.36704600 1.13251500 -0.46058400
H 1.66298900 1.16806600 -1.37987700
C -1.71322100 -0.10657700 -0.11368600
O -0.92625800 -0.94681600 -0.49582600
O -1.44129500 1.16959200 0.14684300
H -0.48812400 1.28032100 -0.00931200
O -3.01900600 -0.32503000 0.11342600
H -3.16236700 -1.25615200 -0.09600700

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Structure 16,IIe:as+as
C 2.05441200 0.07740900 0.02955400
O 1.40314600 0.99261800 0.47593300
O 3.35999700 0.17053600 -0.22156900
H 3.66039400 -0.67770000 -0.57101700
O 1.58320000 -1.14803900 -0.27622100
H 0.63386100 -1.15225100 -0.06767500
C -2.16075300 0.16033100 -0.05062800
O -2.35832400 1.23472700 -0.53890600
O -3.05076600 -0.84495700 -0.04734700
H -2.68256700 -1.57208100 0.46773600
O -1.00913700 -0.22559300 0.57044700
H -0.39857800 0.54125300 0.59870100

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Structure 17,IIf:as+as
C 2.16091700 0.16029200 -0.05058900
O 2.35871800 1.23467600 -0.53880000

O 3.05077300 -0.84513000 -0.04722200
H 2.68241800 -1.57219100 0.46784500
O 1.00914900 -0.22547400 0.57031100
H 0.39875300 0.54150500 0.59856000
C -2.05455700 0.07745400 0.02949900
O -1.40336100 0.99284000 0.47561800
O -3.36021300 0.17031900 -0.22136900
H -3.66053400 -0.67802700 -0.57062400
O -1.58319100 -1.14795600 -0.27620900
H -0.63379900 -1.15196800 -0.06787000

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Structure 18,IIIg:as+as
C 1.82292000 0.14945100 0.06066900
O 1.18312600 1.07562500 -0.37654100
O 1.55556400 -0.44741800 1.21908100
H 2.18524800 -1.16738100 1.34990900
O 2.89371200 -0.39920100 -0.54629600
H 3.01050000 0.07588600 -1.37950100
C -2.05226900 -0.04255600 -0.05258000
O -3.21249900 -0.33502600 0.07263200
O -1.52445000 1.13230300 0.26191400
H -0.56870400 1.13020600 0.06297900
O -1.10343700 -0.89827300 -0.54546500
H -1.58706900 -1.70415200 -0.76452000

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Structure 19,IIIh:as+as
C -1.82269400 0.14942300 0.06069000
O -1.18323900 1.07565200 -0.37688300
O -1.55477100 -0.44723700 1.21908100
H -2.18439700 -1.16717600 1.35036000
O -2.89363200 -0.39949700 -0.54577100
H -3.01087100 0.07549100 -1.37896900
C 2.05200400 -0.04255100 -0.05260900
O 3.21216100 -0.33521500 0.07292100
O 1.52427700 1.13235800 0.26185100
H 0.56856300 1.13039000 0.06277000
O 1.10320500 -0.89806000 -0.54591100
H 1.58683300 -1.70394700 -0.76494700

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Structure 20,IIg:aa+as
C 2.20445800 0.12040600 -0.00430200
O 2.73477600 1.11683800 -0.42428800

O 2.70447400 -1.12097800 -0.01745200
H 3.57433900 -1.05271200 -0.43146200
O 0.98480200 0.06648600 0.57032700
H 0.60501600 0.95700800 0.52614800
C -2.28519200 -0.08401200 -0.06556800
O -3.46327300 -0.09209400 -0.29008500
O -1.50274400 -1.15716900 -0.03621500
H -0.59168800 -0.89395600 0.17661600
O -1.56903400 1.06108700 0.19580500
H -2.21527000 1.77792500 0.16318800

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Structure 21,IIh:as+as
C -2.29824100 -0.06198800 -0.06183800
O -3.48253700 -0.01803200 -0.24689900
O -1.56419100 -1.16770700 -0.04831700
H -0.63603200 -0.94706300 0.13874200
O -1.52484200 1.05473100 0.16341600
H -2.14343000 1.79610300 0.14994500
C 2.21925000 -0.12053000 0.02757500
O 2.82801300 -1.14242100 -0.10826100
O 0.97050200 -0.05237300 0.53159500
H 0.64296000 0.85830300 0.49362000
O 2.65584200 1.12214400 -0.28383400
H 3.54815400 1.01702800 -0.63832900

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Structure 22,IIi:as+as
C -2.21914100 -0.12055300 0.02755700
O -2.82778400 -1.14244500 -0.10880300
O -0.97045600 -0.05248800 0.53177800
H -0.64298800 0.85820800 0.49413000
O -2.65573700 1.12220000 -0.28353300
H -3.54791700 1.01716100 -0.63837000
C 2.29811500 -0.06196800 -0.06185300
O 3.48237800 -0.01799200 -0.24714000
O 1.56413900 -1.16772700 -0.04785100
H 0.63596900 -0.94700200 0.13916400
O 1.52469400 1.05477400 0.16322800
H 2.14322000 1.79618600 0.14941500

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Structure 23,IVa:aa+ss
C 1.80487800 -0.01749800 -0.00056000
O 1.12436800 0.86844700 0.50227900

O 3.07217500 0.13828200 -0.37005000
H 3.30189000 1.05364400 -0.16318200
O 1.41512400 -1.25438200 -0.25706400
H 0.48762000 -1.34235500 0.03108700
C -2.00807400 0.01633900 -0.04027000
O -2.97723500 -0.48716100 -0.51740800
O -1.17991500 -0.67832700 0.81771100
H -0.61887500 -0.04486400 1.28741100
O -1.61201600 1.28032200 -0.28832400
H -0.69146200 1.40308500 -0.00747900

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Structure 24,IVb:aa+ss
C -1.80476800 -0.01743000 -0.00039400
O -1.12447900 0.86855600 0.50267000
O -1.41486100 -1.25428700 -0.25679200
H -0.48748800 -1.34227200 0.03168700
O -3.07190400 0.13803200 -0.37058400
H -3.30192600 1.05337300 -0.16395800
C 2.00794000 0.01635100 -0.04036700
O 2.97701100 -0.48712600 -0.51770900
O 1.61180500 1.28033300 -0.28828100
H 0.69127000 1.40301900 -0.00731200
O 1.17993700 -0.67835500 0.81775500
H 0.61904800 -0.04487500 1.28767800

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Structure 25,IIj:as+as
C 2.19010200 0.15455000 -0.03950100
O 2.48092300 1.22189600 -0.49520300
O 2.94402700 -0.94646000 -0.13233000
H 2.50978100 -1.66068800 0.34902100
O 1.03729500 -0.11162000 0.65031800
H 0.53419400 0.71823500 0.68988800
C -2.26057800 -0.07649900 -0.07156700
O -3.42752000 0.00083400 -0.32935900
O -1.53083100 -1.18853100 -0.13820700
H -0.61557700 -0.98927300 0.11397600
O -1.49349900 0.98822500 0.33916200
H -2.08870100 1.74866900 0.35847100

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Structure 26,IVc:as+ss
C -1.79729900 0.04471500 0.02278500
O -1.10399500 0.91167600 0.51647300

O -3.05165200 0.26862300 -0.35410100
H -3.41059600 -0.55250000 -0.71500200
O -1.42482500 -1.22043000 -0.21088400
H -0.50043800 -1.32756200 0.08390600
C 1.99893900 -0.00444900 -0.04724900
O 2.94437800 -0.55413900 -0.52185400
O 1.15939800 -0.64833600 0.83765600
H 0.59921600 0.01094400 1.27305800
O 1.64686800 1.26584400 -0.32562900
H 0.74060800 1.44162500 -0.02845300

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Structure 27,IVd:as+ss
C 1.79743300 0.04462600 0.02293400
O 1.10391100 0.91109300 0.51718800
O 3.05163200 0.26918000 -0.35401900
H 3.41080800 -0.55160500 -0.71545700
O 1.42534300 -1.22049600 -0.21140500
H 0.50108000 -1.32820400 0.08354200
C -1.99912200 -0.00447100 -0.04717600
O -2.94494100 -0.55411600 -0.52109100
O -1.64713500 1.26575200 -0.32619200
H -0.74111400 1.44205700 -0.02865100
O -1.15918100 -0.64818700 0.83736500
H -0.59767500 0.01101300 1.27124900

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Structure 28,Va:as+ss
C 2.04223000 0.01018700 0.05043500
O 0.98185400 -0.34832900 0.51450700
O 2.26771400 1.24995700 -0.36176300
H 3.17348100 1.31338200 -0.69230300
O 3.11675400 -0.77705200 -0.10225500
H 2.87845800 -1.65530600 0.22391100
C -2.32526900 -0.00125600 -0.04298800
O -3.48450700 0.13058600 -0.30567700
O -1.67795700 -1.18369200 -0.21717100
H -0.75821300 -1.11266000 0.06579300
O -1.57159400 1.01212200 0.44616200
H -0.65360300 0.73225600 0.56748800

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Structure 29,VIa:as+ss
C -1.95195500 -0.10470000 -0.00481700
O -1.28656500 -1.07720000 -0.25864700

O -1.41035600 1.02586800 0.47327100
H -2.09140100 1.70312800 0.57998000
O -3.27872800 0.00898200 -0.14746200
H -3.60089700 -0.83480900 -0.49268700
C 2.20387800 0.00226400 -0.02320100
O 3.39849300 0.03542000 -0.06744100
O 1.44045100 1.05615300 -0.42471300
H 0.54227500 0.98173000 -0.08099500
O 1.51771100 -1.07272800 0.42703000
H 0.59043400 -1.04738400 0.14550500

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Structure 30,VIb:aa+ss
C -2.13731900 -0.00000100 0.00001300
O -3.33593500 -0.00015900 -0.00024800
O -1.32824500 0.98918100 -0.43253100
H -1.89321400 1.72271800 -0.71063400
O -1.32813400 -0.98896000 0.43284200
H -1.89287200 -1.72269000 0.71093000
C 2.18410900 -0.00001800 -0.00005700
O 3.37919700 -0.00006400 -0.00014400
O 1.45780000 -1.00931800 -0.54625400
H 0.54197700 -0.98149100 -0.24152400
O 1.45797800 1.00931900 0.54629300
H 0.54207700 0.98158600 0.24182300

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Structure 31,VIc:aa+ss
C 2.13691300 -0.00020000 0.00014400
O 3.33551800 0.00065700 -0.00174200
O 1.32851300 -0.98895600 0.43483500
H 1.89371300 -1.72235900 0.71243500
O 1.32700800 0.98848500 -0.43209400
H 1.89181500 1.72157200 -0.71136700
C -2.18375600 -0.00007000 -0.00061500
O -3.37881300 -0.00212300 -0.00034900
O -1.45902400 1.00932900 0.54733100
H -0.54362100 0.98348000 0.24147700
O -1.45575300 -1.00763700 -0.54769600
H -0.54043700 -0.97910700 -0.24199400

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Structure 32,Vb:aa+ss
C -2.08263700 0.08021900 -0.00306300
O -3.28094800 0.02354200 -0.00912700

O -1.24448600 -0.99500500 0.03675800
H -1.80376600 -1.78359600 0.06224300
O -1.30480600 1.16433900 -0.03233400
H -1.88896800 1.93351800 -0.06374500
C 2.11685200 -0.00254200 -0.00139000
O 3.22163100 0.45187000 -0.02316200
O 1.44985800 -0.33534000 -1.13643100
H 0.56109100 -0.64914000 -0.93351900
O 1.45444700 -0.23600600 1.16088500
H 0.56078700 -0.55403500 0.98902400

****

Structure 33,IIIi:as+ss
C -1.94854100 -0.06020500 -0.05452900
O -3.09155200 -0.39083800 0.11916100
O -1.46915900 1.15880400 0.13889900
H -0.52175600 1.19381000 -0.09498800
O -0.97115700 -0.92525900 -0.48389600
H -1.43767400 -1.75130500 -0.66292400
C 1.74644300 0.18863800 0.01358400
O 1.24281500 1.12362200 -0.54560900
O 1.40386600 -0.15577100 1.27808000
H 1.47203800 -1.11029800 1.39183900
O 2.69950200 -0.56578200 -0.56775400
H 3.18546500 -1.06101400 0.10069400

****

Structure 34,IIIj:as+ss
C 1.94847800 -0.05984200 -0.05487600
O 3.09086700 -0.39061800 0.12250300
O 1.46815000 1.15870700 0.13916800
H 0.52167300 1.19382200 -0.09814200
O 0.97274600 -0.92409000 -0.48945500
H 1.43983300 -1.74970300 -0.66894600
C -1.74670500 0.18816800 0.01438000
O -1.24447600 1.12355500 -0.54550100
O -1.40026500 -0.15742600 1.27741800
H -1.46916600 -1.11184100 1.39123500
O -2.70156600 -0.56536500 -0.56483100
H -3.18661700 -1.06033500 0.10441000

****

Structure 35,IVe:as+ss
C 1.99832300 -0.10198200 -0.09047200
O 3.13504200 0.09835100 -0.40378100

O 1.35031200 -1.25078900 -0.20476600
H 0.45417500 -1.18466100 0.17091600
O 1.18571700 0.89007900 0.45295000
H 1.76851700 1.65639800 0.54908600
C -2.00845400 0.00888600 -0.05077400
O -2.94990600 -0.52496700 -0.54441400
O -1.21156500 -0.63303500 0.88559300
H -0.81726600 0.03158600 1.46536600
O -1.59552600 1.25945100 -0.33903900
H -0.65724500 1.34253400 -0.11023600

****

Structure 36,IVf:as+ss
C -1.99839300 -0.10198400 -0.09045800
O -3.13524200 0.09803600 -0.40353800
O -1.35018200 -1.25071100 -0.20459200
H -0.45395600 -1.18428400 0.17088500
O -1.18587200 0.89039800 0.45238800
H -1.76867400 1.65674200 0.54832000
C 2.00851200 0.00880500 -0.05072700
O 2.94981000 -0.52520600 -0.54446300
O 1.21144800 -0.63303200 0.88555000
H 0.81752200 0.03176800 1.46536700
O 1.59589000 1.25952800 -0.33875800
H 0.65757400 1.34274700 -0.11015200

****

Structure 37,Vc:as+ss
C 2.16519500 0.14677600 0.00090900
O 2.12777900 1.34142200 0.00876900
O 1.04332100 -0.62243000 -0.00447400
H 1.29355000 -1.55668900 -0.01051500
O 3.25455800 -0.64298700 -0.00396900
H 4.02582300 -0.06037300 0.00008200
C -2.34617300 0.00743900 0.00009100
O -3.54051500 0.01795900 0.00018100
O -1.62254100 -0.00936500 1.14965500
H -0.67699500 -0.02306200 0.96085700
O -1.62254100 0.00606100 -1.14959200
H -0.67699500 -0.01045100 -0.96099000

****

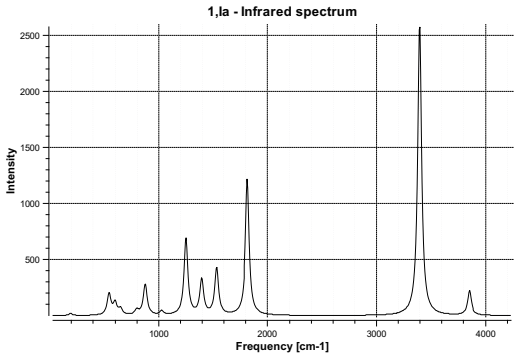
Structure 38,IIk:as+ss
C -2.24295100 -0.05072400 -0.05771200
O -3.41537900 0.00886400 -0.29877800

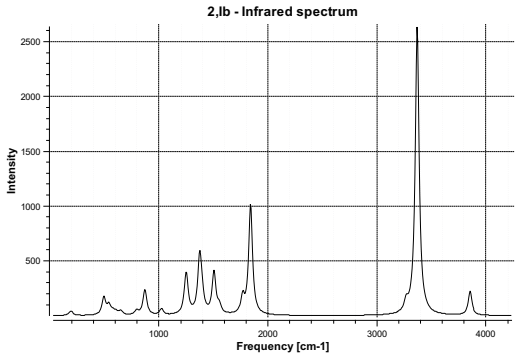
O -1.55693300 -1.16175600 0.16574300
H -0.62133800 -0.95687000 0.33856100
O -1.43601200 1.07034600 0.02047800
H -2.02768400 1.81349800 -0.15468200
C 2.17875300 -0.14682100 -0.01489200
O 2.61400000 -1.21062000 -0.32490100
O 2.82253500 1.02110600 -0.24958200
H 2.46540000 1.72000500 0.30864100
O 0.97450600 -0.00667400 0.62703400
H 0.54707700 0.83850500 0.42314400

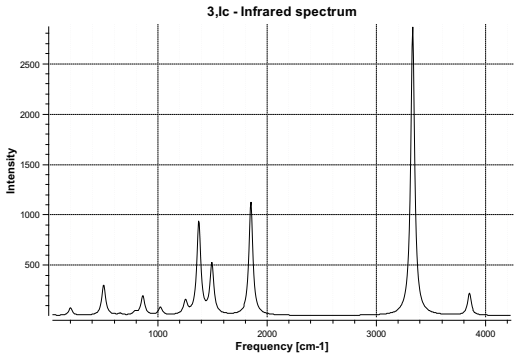
****
Structure 39,Vd:ss+ss
C 2.29797100 -0.00001400 -0.07048600
O 3.43705700 0.00358200 -0.43701600
O 1.61119600 1.14675200 0.15717600
H 0.70391300 0.96128900 0.43451700
O 1.61431200 -1.15196600 0.14245500
H 0.70740900 -0.97266700 0.42472700
C -2.01154600 0.00026900 0.08760200
O -0.95061600 -0.00366000 0.65784700
O -2.62295800 -1.15025700 -0.23583700
H -3.48973200 -1.01324700 -0.63267500
O -2.61656300 1.15539000 -0.23232300
H -3.41957100 1.02437100 -0.74768400

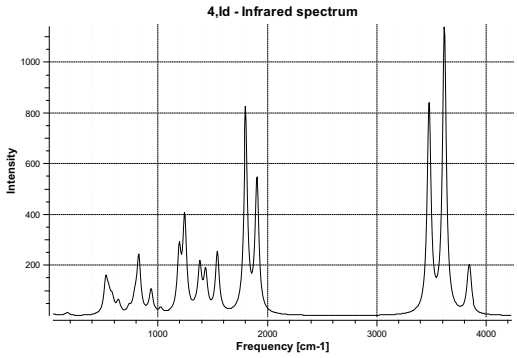
****
Structure 40,VId:ss+ss
C 1.97309000 -0.14381600 0.00029100
O 1.23499300 -1.08154800 -0.10973000
O 1.50717800 1.05017800 0.46274000
H 2.07966600 1.78922900 0.22555700
O 3.27599200 -0.20624400 -0.31053900
H 3.76551100 0.53690600 0.05868100
C -2.22324500 0.02013700 -0.03392200
O -3.40962200 0.11932900 -0.14604800
O -1.38965300 1.06980900 -0.28221900
H -0.50908300 0.90472500 0.07375500
O -1.61510400 -1.12462500 0.34704200
H -0.66543200 -1.10397200 0.15381900
****

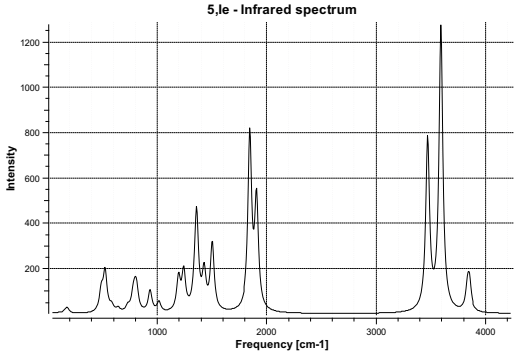
2 MP2/6–311++G** calculated IR spectra for the five most stable dimers










5,le - Infrared spectrum
Intensity
1200
1000
800
600
400
200
1000
2000
3000
4000
Frequency [cm-1]