Electronic Supplementary Material (ESI) for ChemComm.

On the Encapsulation of Hydrocarbon Components of Natural Gas within Molecular Baskets in Water. The Role of C–H···π Interactions and the Host's Conformational Dynamics in the Process of Encapsulation

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Supplementary Information

^{1}H NMR Titrations Experiments

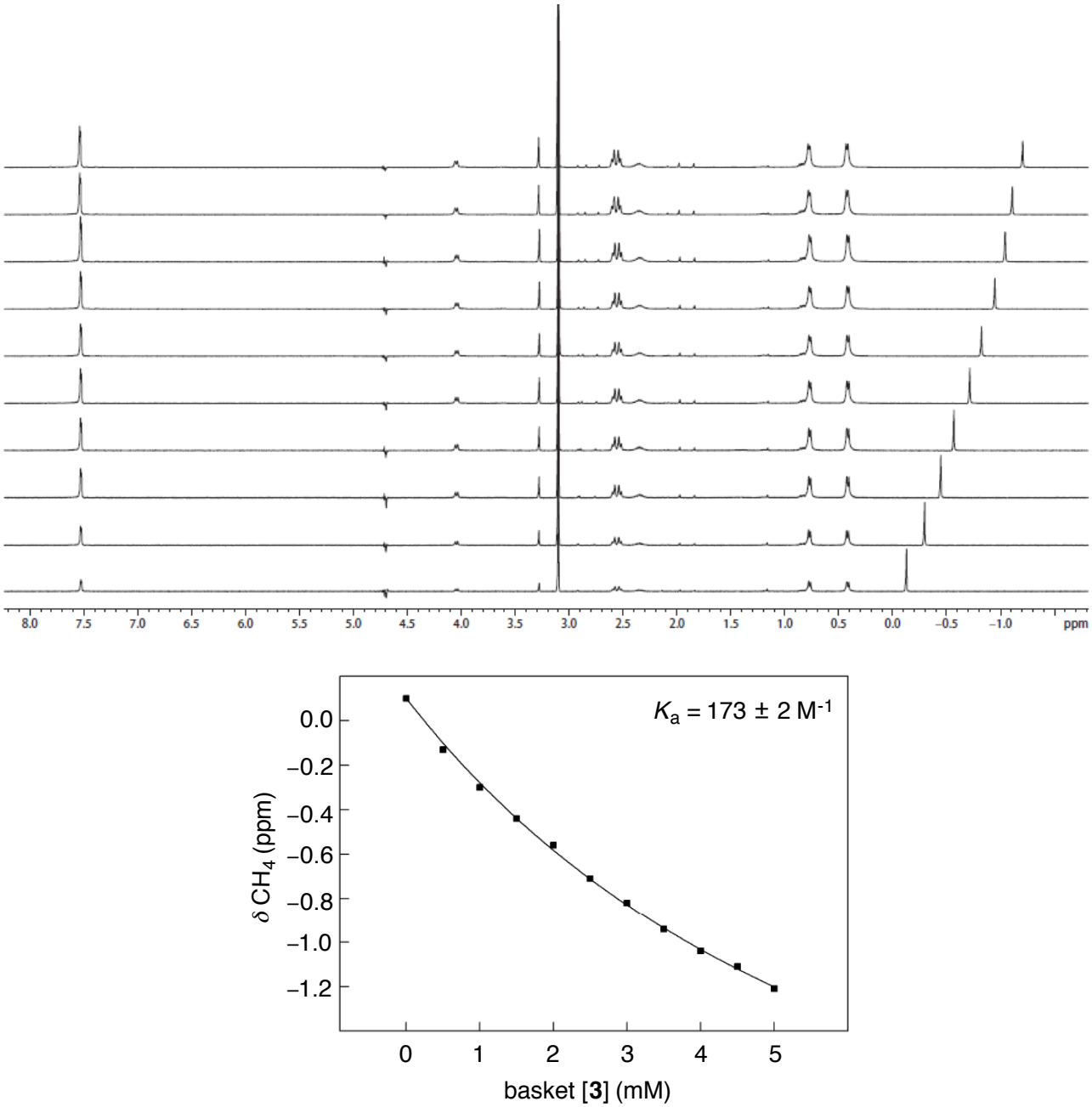

Figure S1. (Top) ^{1}H NMR spectra (400 MHz, 298.2 K) obtained upon an incremental addition of basket [**3**] (from 0.5 to 5.0 mM) to a saturated solution of methane (1.3 mM) in phosphate buffer (10.0 mM) at pH = 7.0 ± 0.1. (Bottom) Nonlinear least-square analysis of the binding data (1:1 binding stoichiometry) gave the apparent association constant K_{app} = 173 ± 2 M^{-1} (R^2 = 0.999, SigmaPlot) for the formation of [**3**–CH_4].

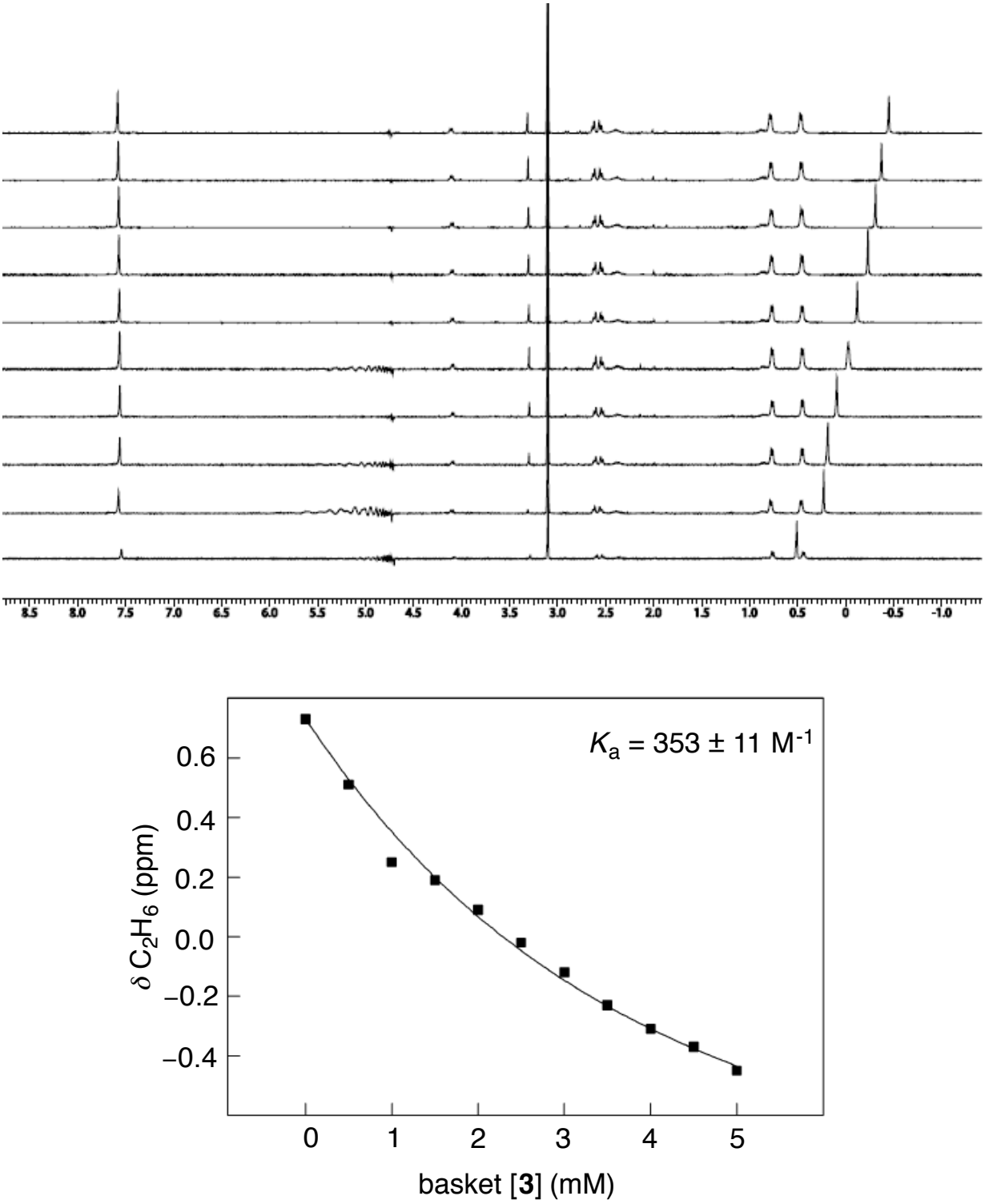

Figure S2. (Top) ^{1}H NMR spectra (400 MHz, 298.2 K) obtained upon an incremental addition of basket [**3**] (from 0.5 to 5.0 mM) to a saturated solution of ethane (1.8 mM) in phosphate buffer (10.0 mM) at pH = 7.0 ± 0.1. (Bottom) Nonlinear least-square analysis of the binding data (1:1 binding stoichiometry) gave the apparent association constant K_{app} = 353 ± 11M^{-1} (R^2 = 0.991, SigmaPlot) for the formation of [**3–**C_2H_6].

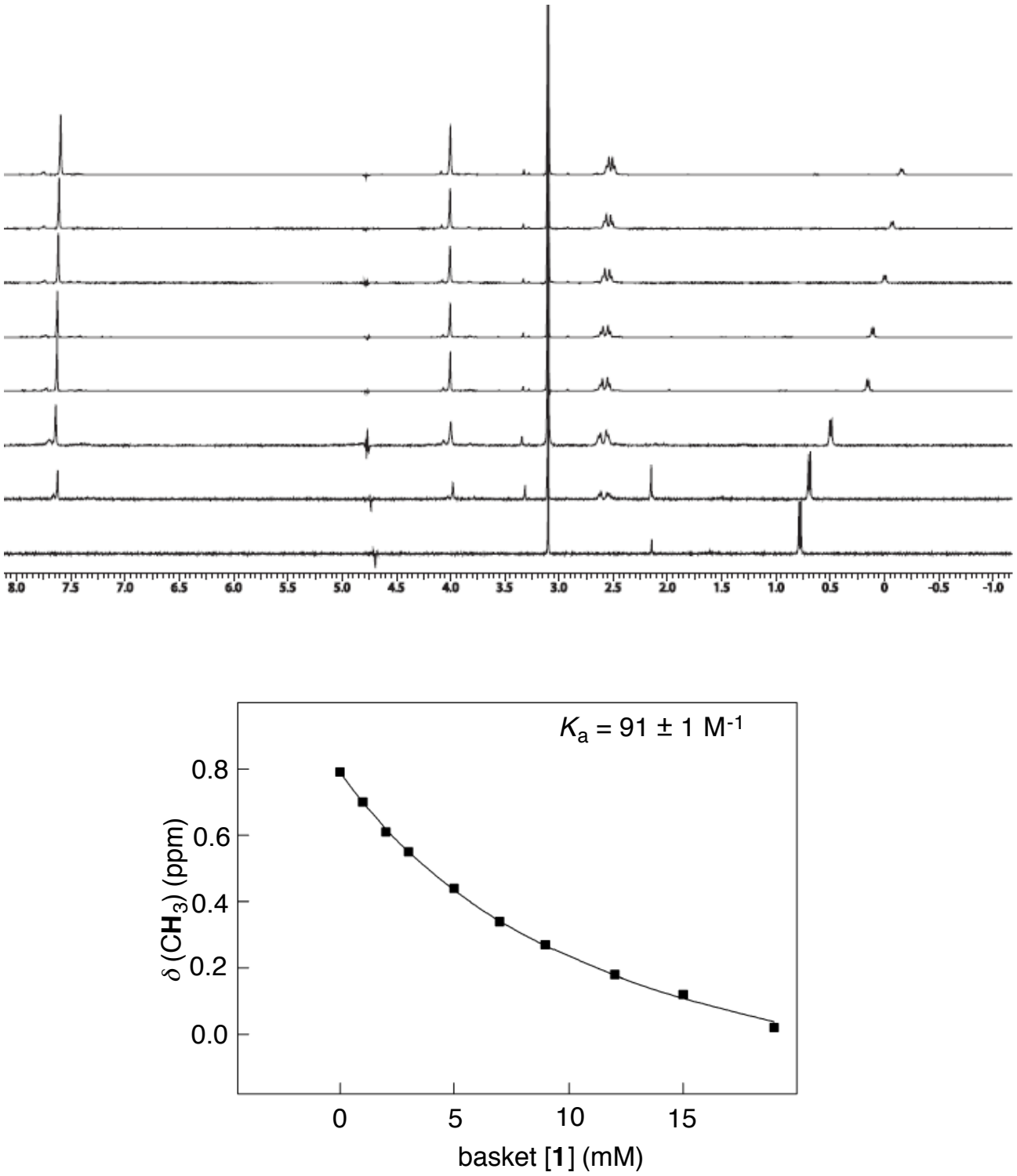

Figure S3. (Top) ^{1}H NMR spectra (400 MHz, 298.2 K) obtained upon an incremental addition of basket [**1**] (from 1.0 to 15.0 mM) to a saturated solution of propane (1.4 mM) in phosphate buffer (10.0 mM) at pH = 7.0 ± 0.1. (Bottom) Nonlinear least-square analysis of the binding data (1:1 binding stoichiometry) gave the apparent association constant K_{app} = 91 ± 1 M^{-1} (R^2 = 0.999, SigmaPlot) for the formation of [**1**–C_3H_8].

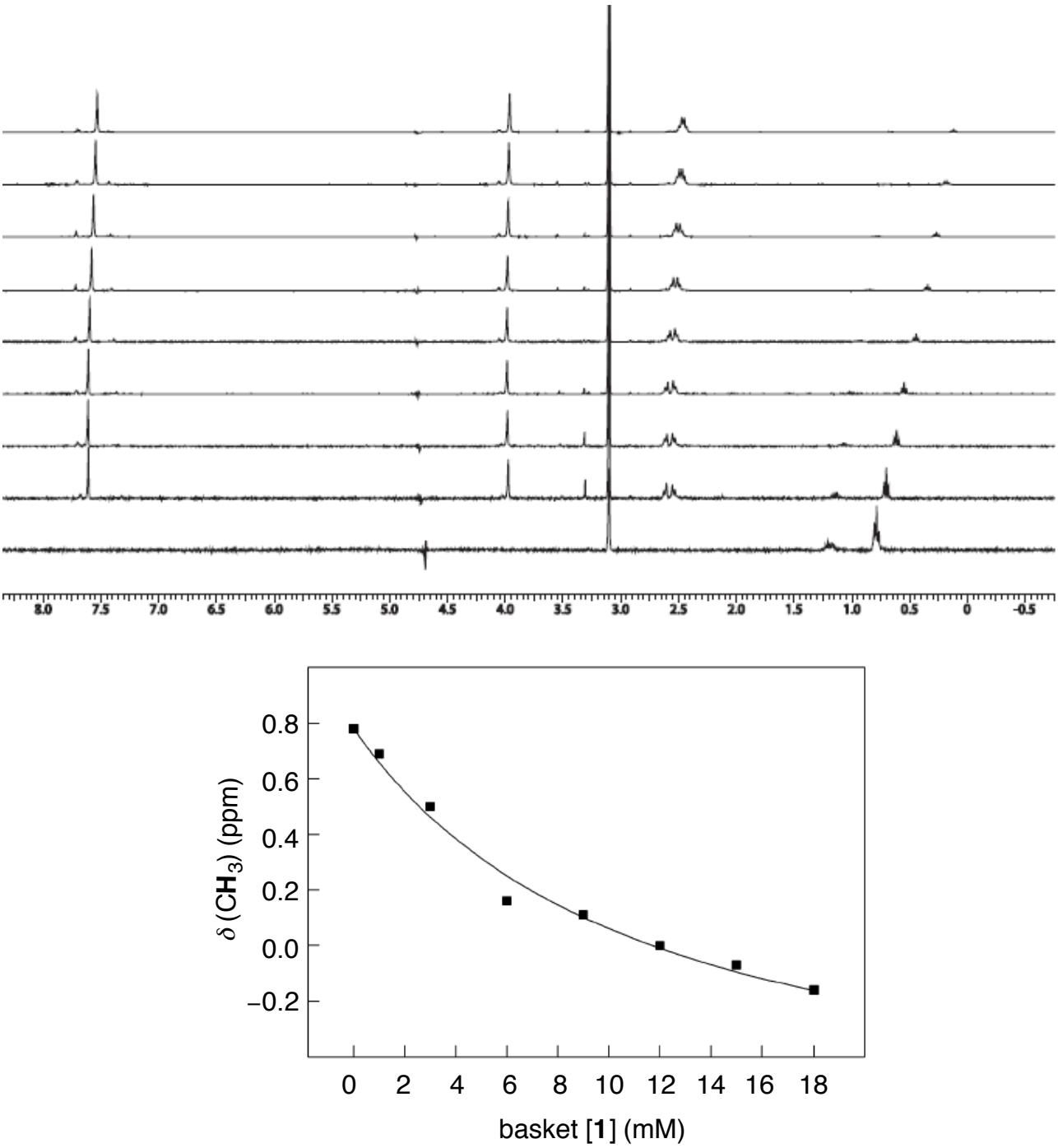

Figure S4. (Top)^{1}H NMR spectra (400 MHz, 298.2 K) obtained upon an incremental addition of basket [**1**] (from 1.0 to 18.0 mM) to a saturated solution of isobutane (0.8 mM) in phosphate buffer (10.0 mM) at pH = 7.0 ± 0.1. (Bottom) Nonlinear least-square analysis of the binding data (1:1 binding stoichiometry) gave the apparent association constant K_{app} = 93 ± 4 M^{-1} (R^2 = 0.987, SigmaPlot) for the formation of [**1**–C_4H_{10}].

Diffusion NMR Experiments

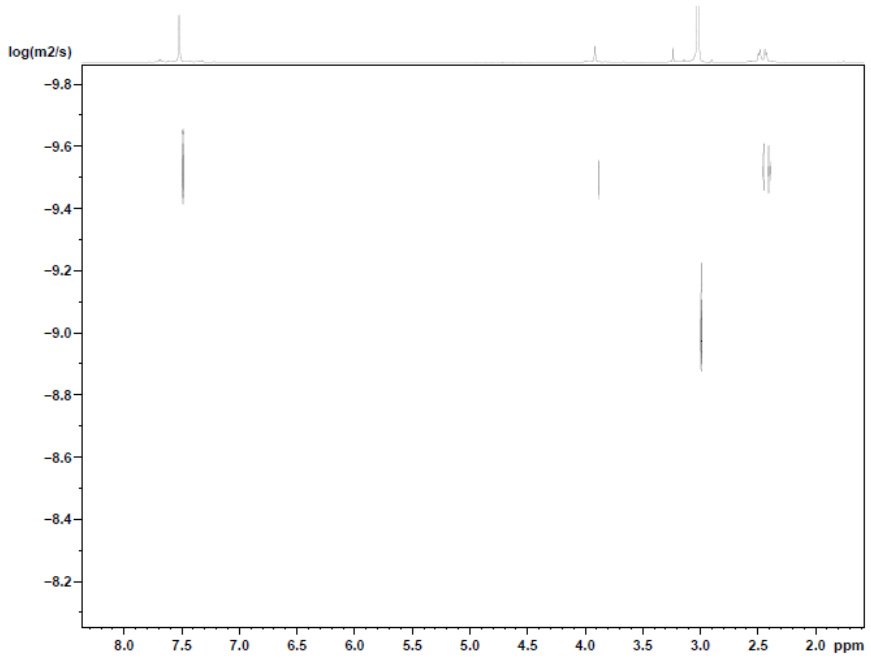

Figure S5. DOSY NMR spectrum (600MHz, 298.2 K) of basket [**3**] (4.0mM) in phosphate buffer (10.0mM, pH = 7.0 ± 0.1).

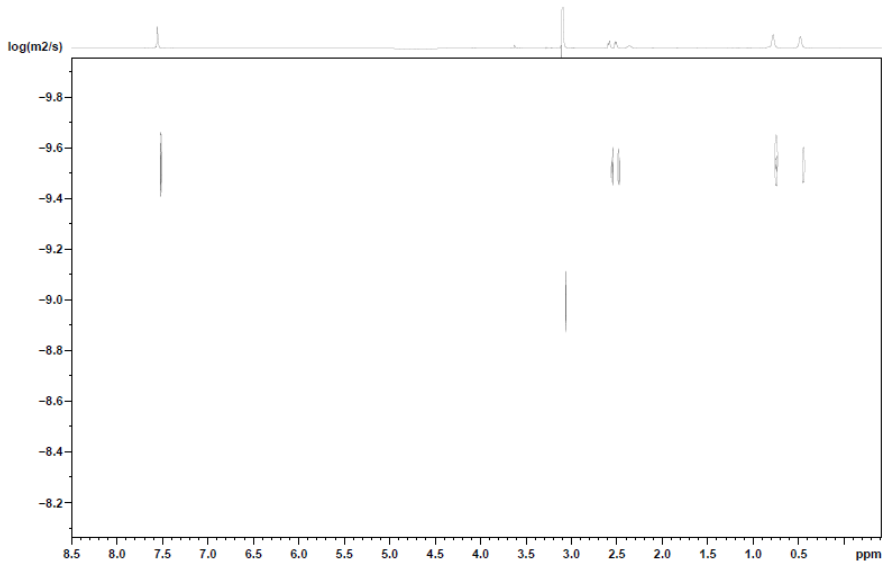

Figure S6. DOSY NMR spectrum (600MHz, 298.2 K) of basket [**1**] (10.0mM) in phosphate buffer (10.0mM, pH = 7.0 ± 0.1).

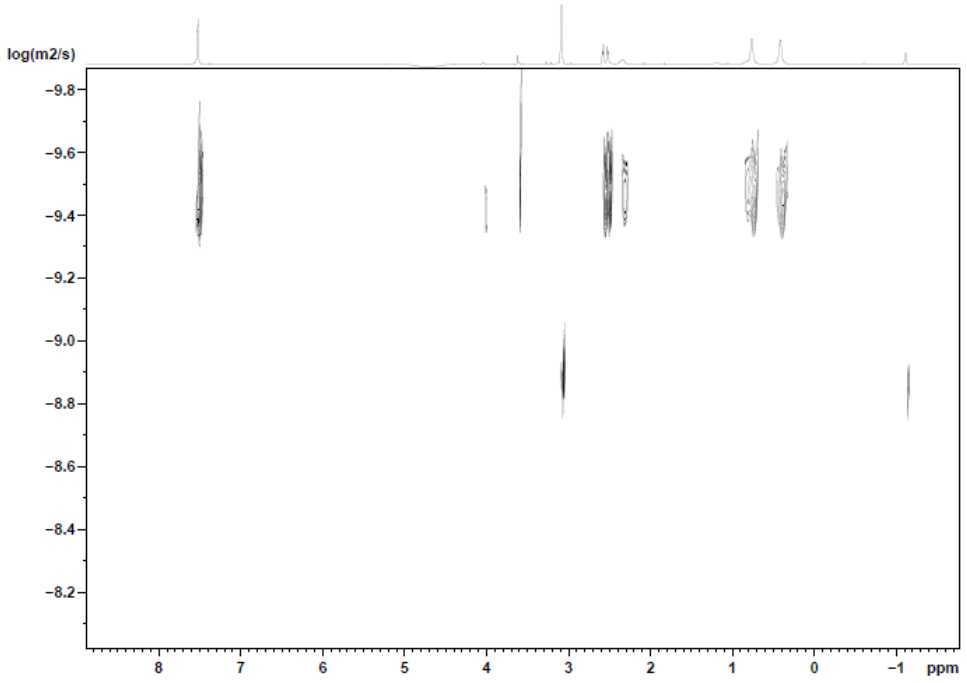

Figure S7. DOSY NMR spectrum (600MHz, 298.2 K) of basket [**3**] (4.0mM) and methane (1.3 mM) in phosphate buffer (10.0mM, pH = 7.0 ± 0.1).

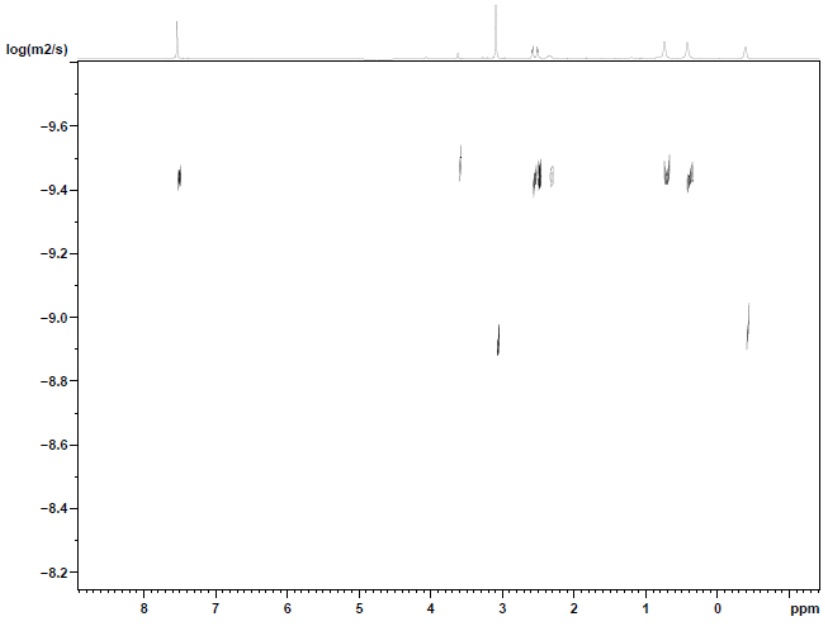

Figure S8. DOSY NMR spectrum (600MHz, 298.2 K) of basket [**3**] (4.0mM) and ethane (1.8 mM) in phosphate buffer (10.0mM, pH = 7.0 ± 0.1).

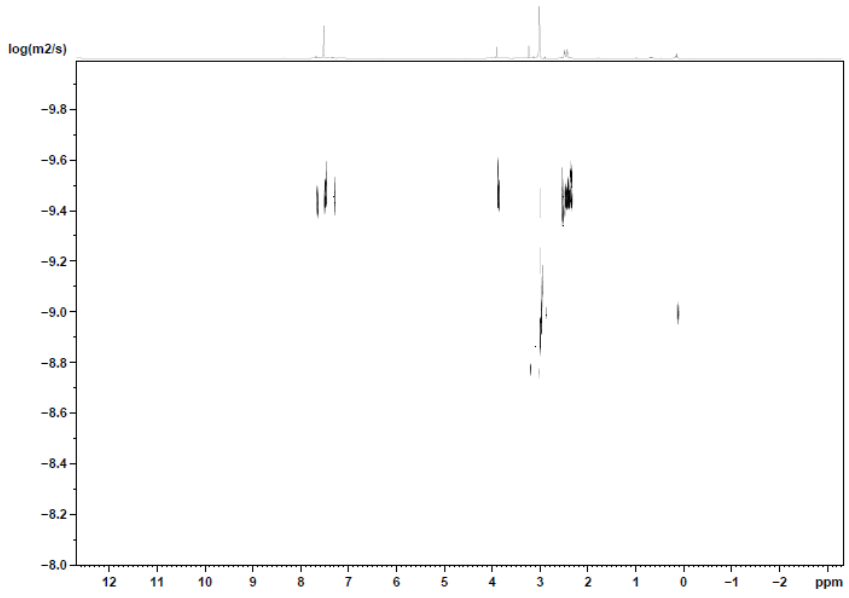

Figure S9. DOSY NMR spectrum (600MHz, 298.2 K) of basket [**1**] (10.0mM) and propane (1.4 mM) in phosphate buffer (10.0mM, pH = 7.0 ± 0.1).

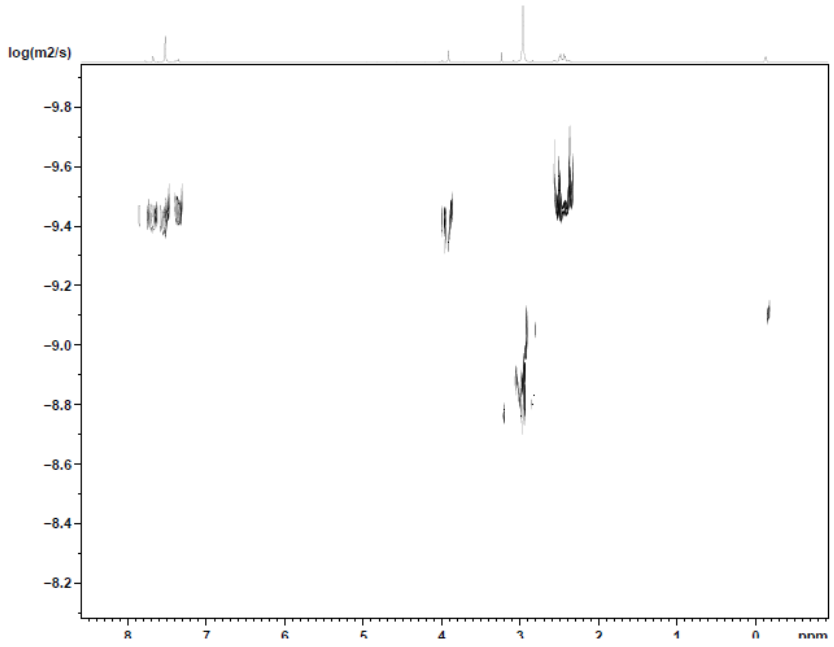

Figure S10.DOSY NMR spectrum (600MHz, 298.2 K) of basket [**1**] (10.0mM) and isobutane (0.8 mM) in phosphate buffer (10.0mM, pH = 7.0 ± 0.1).

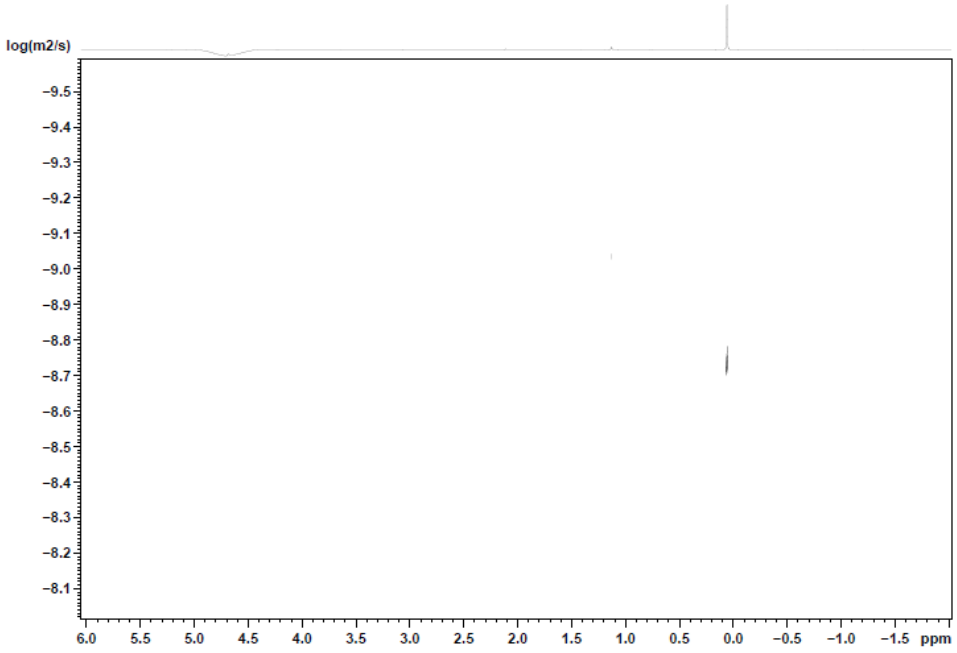

Figure S11. DOSY NMR spectrum (600MHz, 298.2 K) of methane (1.3 mM) in phosphate buffer (10.0mM, pH = 7.0 ± 0.1).

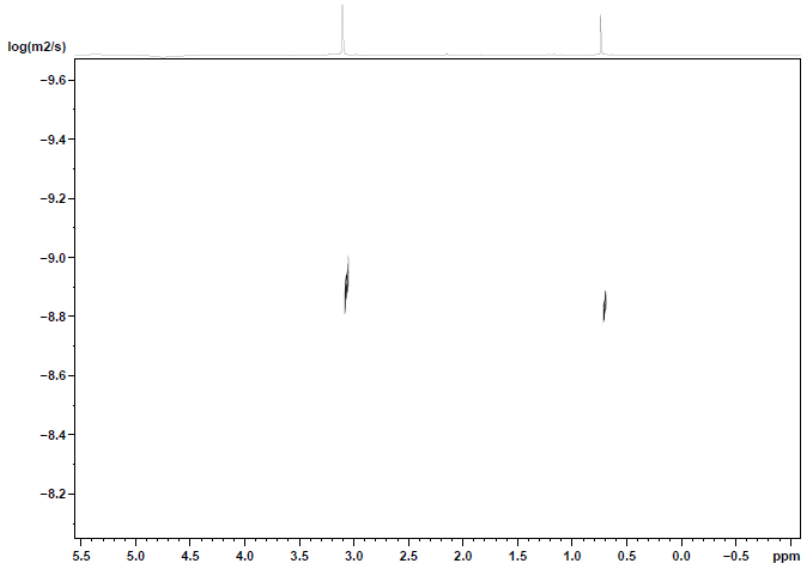

Figure S12. DOSY NMR spectrum (600MHz, 298.2 K) of ethane (1.8 mM) in phosphate buffer (10.0mM, pH = 7.0 ± 0.1).

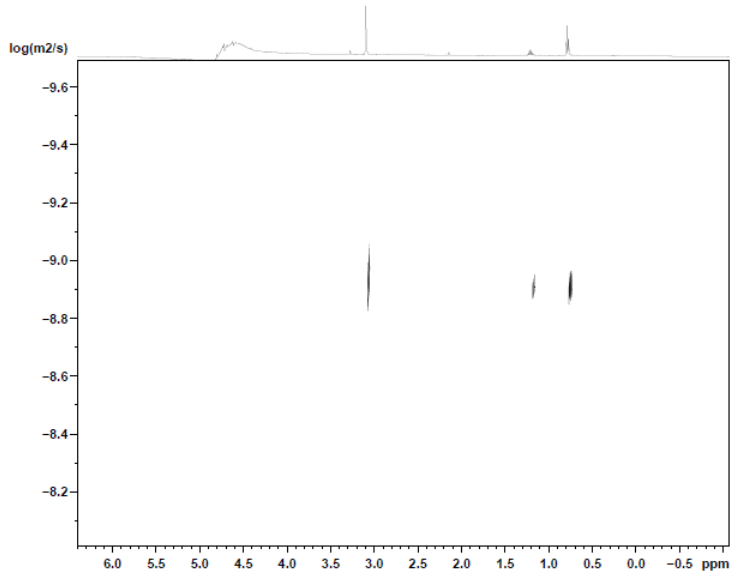

Figure S13. DOSY NMR spectrum (600MHz, 298.2 K) of propane (1.4 mM) in phosphate buffer (10.0mM, pH = 7.0 ± 0.1).

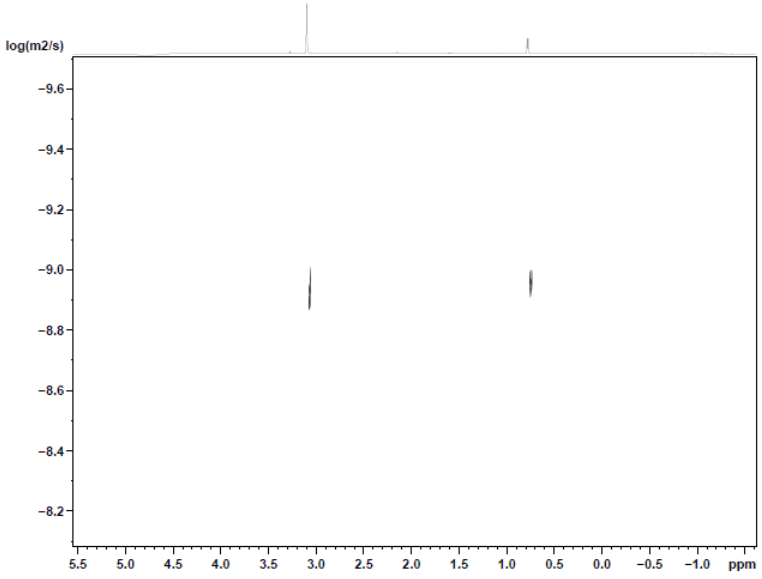

Figure S14. DOSY NMR spectrum (600MHz, 298.2 K) of methane (0.8 mM) in phosphate buffer (10.0mM, pH = 7.0 ± 0.1).

^{1}H NMR Study of Basket [3] and Alcohols (CH_3OH, C_2H_5OH, *iso*-C_3H_7OH and *tert*-C_4H_9OH) in Water

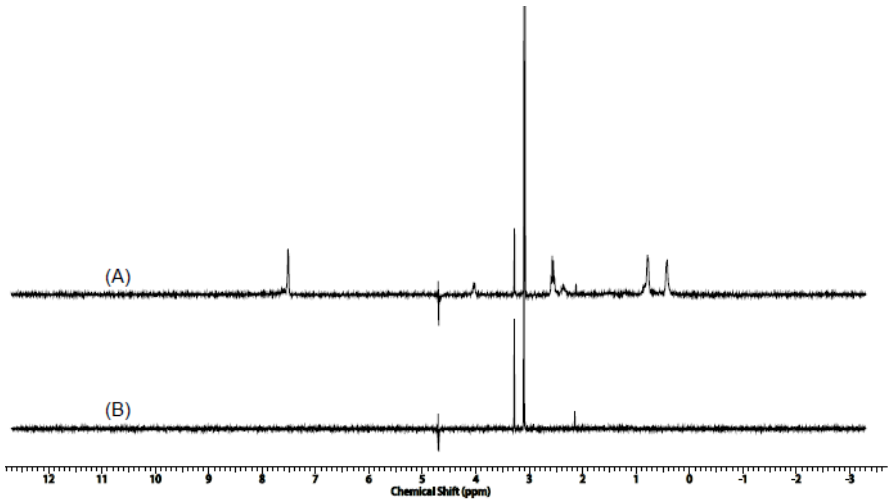

Figure S15. (**A**) ^{1}H NMR spectrum (400 MHz, 300.2 K) of basket [**3**] (1.0 mM) and methanol (0.7 mM) in aqueous phosphate buffer (10.0 mM) at pH = 7.0 ± 0.1. ^{1}H NMR signals at 4.7 ppm are missing because of the suppression of water's resonance. (**B**) ^{1}H NMR spectrum (400 MHz, 300.2 K) of methanol (0.7 mM) in aqueous phosphate buffer (10.0 mM) at pH = 7.0 ± 0.1. Note that ^{1}H NMR resonance at δ = 3.28 ppm corresponding to CH_3 nuclei in methanol stayed unperturbed; $(CH_3)_4NBr$ (δ = 3.1 ppm) served as an internal standard in both **A** and **B**.

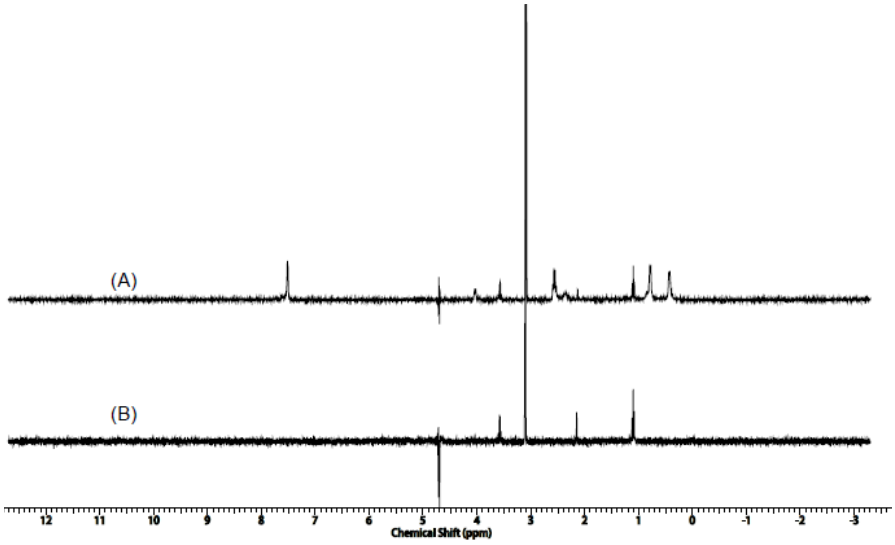

Figure S16. (**A**) ^{1}H NMR spectra (400 MHz, 300.2 K) of basket [**3**] (1.0 mM) and ethanol (0.8 mM) in aqueous phosphate buffer (10.0 mM) at pH = 7.0 ± 0.1. ^{1}H NMR signals at ~ 4.7 ppm are missing because of the suppression of the water's resonance. (**B**) ^{1}H NMR spectrum (400 MHz, 300.2 K) of ethanol (0.8mM)in aqueous phosphate buffer (10.0 mM) at pH = 7.0 ± 0.1. Note that ^{1}H NMR resonance at δ = 1.10 ppm corresponding to CH_3 nuclei in ethanol stayed unperturbed; $(CH_3)_4NBr$ (δ = 3.1 ppm) served as an internal standard in both **A** and **B**.

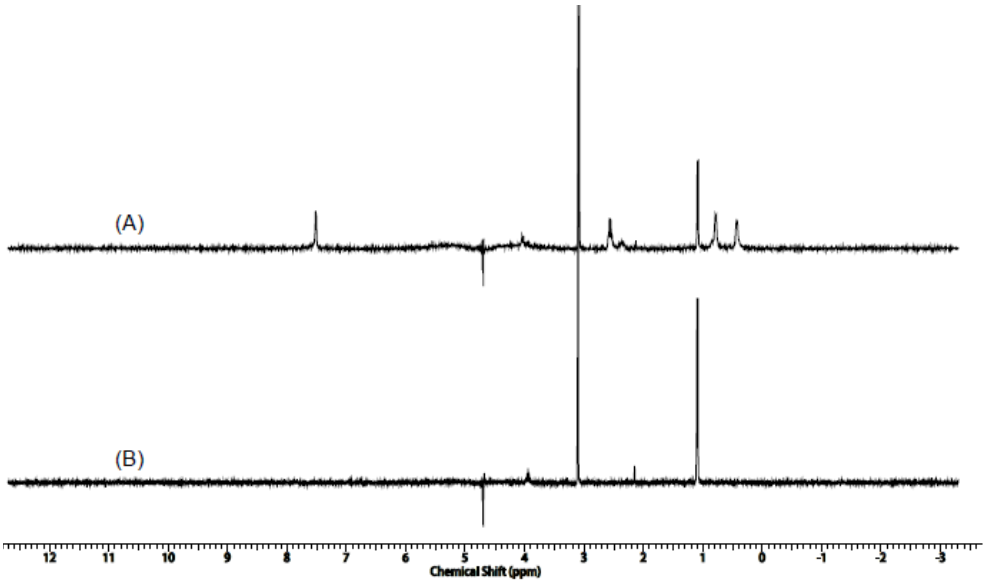

Figure S17. (**A**) ^{1}H NMR spectra (400 MHz, 300.2 K) of basket [**3**] (1.0 mM) and *iso*-propanol (1.1 mM) in aqueous phosphate buffer (10.0 mM) at pH = 7.0 ± 0.1. ^{1}H NMR signals at ~ 4.7 ppm are missing because of the suppression of the water's resonance. (**B**) ^{1}H NMR spectrum (400 MHz, 300.2 K) of *iso*-propanol (1.1 mM)in aqueous phosphate buffer (10.0 mM) at pH = 7.0 ± 0.1. Note that ^{1}H NMR resonance at δ = 1.09 ppm corresponding to CH_3 nuclei in propanol stayed unperturbed; $(CH_3)_4NBr$ (δ = 3.1 ppm) served as an internal standard in both **A** and **B**.

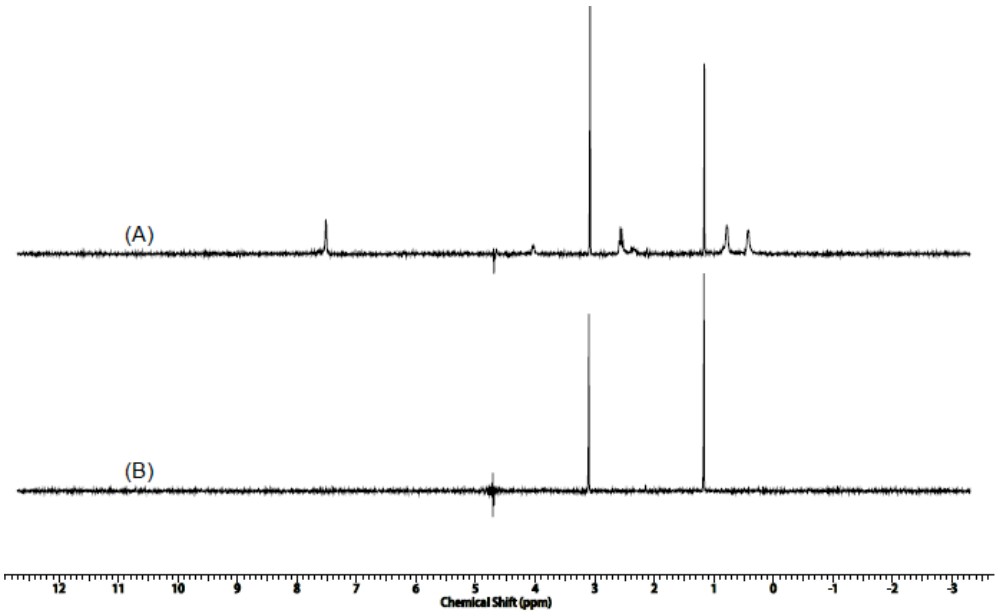

Figure S18. (**A**) ^{1}H NMR spectra (400 MHz, 300.2 K) of basket [**3**] (1.0 mM) and *tert*-butanol (0.9 mM) in aqueous phosphate buffer (10.0 mM) at pH = 7.0 ± 0.1. ^{1}H NMR signals at ~ 4.7 ppm are missing because of the suppression of the water's resonance. (**B**) ^{1}H NMR spectrum (400 MHz, 300.2 K) of *tert*-butanol(0.9 mM)in aqueous phosphate buffer (10.0 mM) at pH = 7.0 ± 0.1. Note that ^{1}H NMR resonance at δ = 1.16 ppm corresponding to CH_3 nuclei in *tert*-butanol stayed unperturbed; $(CH_3)_4NBr$ (δ = 3.1 ppm) served as an internal standard in both **A** and **B**.

Computational Methods

We used Gaussian09 for the geometry optimizations of baskets [**1**], [**2**], [**3**] as well as [**1**–gas], [**2**–gas] and [**3**–gas];[1] note that gas = methane, ethane and propane. The optimizations and frequency calculations were performed at the M062X/6-31G* level of theory. Each structure was fully optimized at the specified level of theory, and then confirmed to be a minimum, with zero imaginary vibrational frequencies, on the potential energy surface by computation of the analytical second derivatives.

Computed Coordinates

Basket [**1**]

C	1.43474700	-0.85778500	3.33706600
C	0.24704400	-1.53631400	3.37551900
C	-0.97869400	-0.81962500	3.47749200
C	-0.96955300	0.54733600	3.53361400
C	0.26562800	1.25339600	3.49062800
C	1.44419700	0.56444300	3.39813200
C	-0.12649500	-3.01570400	3.32310800
H	0.67152400	-3.72742900	3.53677800
C	-2.08842900	-1.86813400	3.48830600
H	-3.06277500	-1.54138800	3.85273300
C	-1.35642600	-2.99304300	4.27590400
H	-1.09682600	-2.69620900	5.29558700
H	-1.90851000	-3.93694600	4.27806100
C	-0.85622300	-3.21046700	1.99746100
C	-2.07241000	-2.50021000	2.09995000
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H	3.14043800	2.00114700	3.65347500
C	3.54452200	-0.19403200	4.11889700
H	4.63689900	-0.19892700	4.06896500
H	3.20592600	-0.23855300	5.15746000
C	3.37926300	0.61234600	1.92542400
C	3.36738200	-0.79818400	1.86110000
C	-2.06510200	1.60696400	3.62739200
H	-3.04459700	1.26569400	3.96355400
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C	-2.98686000	-2.45867200	1.05971400
C	-0.50633600	-3.90597500	0.85118900
C	-2.94529300	2.38740800	1.24735700
C	-0.44814100	3.81817700	1.15616600
C	3.72530100	-1.48262900	0.71049900
C	3.75350700	1.39376400	0.84404500

H	-3.92971300	-1.92298700	1.11927400
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H	-3.89309200	1.85748200	1.26331100
H	0.48634600	4.36881200	1.10331900
H	3.77403400	2.47902600	0.87487500
H	3.72431400	-2.56623600	0.63970800
C	-3.39497800	-3.36742000	-1.35230000
C	-1.39138200	-4.53355200	-1.52066600
N	-2.56230400	-4.13360100	-2.17562200
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O	-0.55158500	-5.26583800	-1.98115000
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C	4.60498200	1.22202600	-1.61590100
N	4.79370400	0.09381900	-2.42292000
O	4.74730000	-2.20573800	-2.17515700
O	4.80434500	2.36025400	-1.95932400
C	5.40169700	0.14615100	-3.72171600
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O	-4.11936400	-6.25763500	-2.02473800
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C	-2.57699400	3.17544200	0.16065600
C	-1.30934900	4.61811900	-1.17244700
C	-3.32635700	3.46529200	-1.09856100
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O	-4.42820000	3.11156500	-1.43672700
N	-2.47884600	4.27603600	-1.86163800
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C	-3.90617300	6.02859900	-2.87784000
O	-4.52111700	6.53487100	-3.77753500
O	-4.00819900	6.40911300	-1.59410900
H	-4.66346900	7.12839400	-1.57198800
H	-3.35137900	4.17610900	-3.75315900
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H	-2.12678700	-5.08898300	-3.94251100

Sum of electronic and zero-point Energies= -2796.415309

Sum of electronic and thermal Energies= -2796.371397

Sum of electronic and thermal Enthalpies= -2796.370453

Sum of electronic and thermal Free Energies -2796.498553

Basket [**1**−CH_4]

C	-0.18247100	-1.24993600	3.68867600
C	-1.36789400	-0.57251200	3.59770700
C	-1.37322300	0.84999700	3.54939900
C	-0.19342000	1.54116500	3.60319300
C	1.03869100	0.83719800	3.71138200
C	1.04410800	-0.53086300	3.74652000
C	-2.82383700	-1.01076700	3.46028700
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C	-2.83216200	1.26654900	3.37845000
H	-3.07293000	2.30452200	3.60982400
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H	-3.22012600	0.19324500	5.28391700
H	-4.59783500	0.14644100	4.12911300

C	-3.22771600	-0.62963200	2.03956100
C	-3.23139000	0.78166800	1.98795000
C	0.19048100	-2.73013700	3.65135000
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C	2.15437900	-1.57821000	3.73742700
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H	1.23012800	-2.39386700	5.58338500
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C	2.14195300	1.89153300	3.65037200
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C	1.42305800	3.05520800	4.38836700
H	1.19127600	2.81671600	5.42973300
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C	2.51821000	-2.81644700	0.11969300
C	1.32299700	-3.52157000	0.06964500
C	-3.84742900	-0.70432300	-0.22684000
C	-3.85200600	0.68316600	-0.27795600
C	-3.53942800	1.47181300	0.82630600
C	-3.53066500	-1.40641100	0.93279500
C	0.43973000	3.68697500	0.91531100
C	2.93817200	2.27325000	1.14660400
C	0.45522100	-3.59443700	1.15547800
C	2.93409200	-2.13211800	1.25856800
H	-3.55405200	2.55616200	0.76507700
H	-3.53750900	-2.49234100	0.95306200
H	-0.50091200	4.21871400	0.80527300
H	3.88249300	1.74071800	1.21118600
H	3.87284800	-1.58616200	1.27461500
H	-0.47624500	-4.14983200	1.09553100
C	-4.25993400	1.09966000	-1.65371800
C	-4.25326800	-1.22382200	-1.56743800
N	-4.41787400	-0.09077800	-2.37341500
O	-4.43261100	2.20663700	-2.09849200
O	-4.42114900	-2.36105000	-1.92915100
C	1.19835200	-4.13842300	-1.28516800
C	3.20292500	-2.96465400	-1.19970800
N	2.32229400	-3.70400400	-1.99815500
O	0.33694100	-4.86143100	-1.71958300
O	4.28256900	-2.56213600	-1.55430400
C	2.67846700	-4.20438200	-3.29552200
H	1.76151600	-4.48283000	-3.82228100
C	3.58495800	-5.42522900	-3.26348900
O	4.07629800	-5.90749800	-4.24827000
O	3.75854400	-5.91285400	-2.02455400
H	4.34048700	-6.68796700	-2.11315600
C	-4.97180900	-0.14140800	-3.69642100
H	-4.64933300	0.74358100	-4.25074100
C	-6.49175100	-0.18099000	-3.73479000
O	-7.12257100	-0.24650500	-4.75555900
O	-7.04739300	-0.13001200	-2.51363000
H	-8.01093600	-0.15850900	-2.64844200
C	2.51648000	2.85178700	-0.04700100
C	1.31141800	3.53278300	-0.15889100
C	3.19682300	2.88403500	-1.37630600
C	1.17830300	4.02164400	-1.56450000
O	4.27918400	2.46022100	-1.69540100
O	0.30684300	4.68996200	-2.06186600

N	2.30652700	3.53686300	-2.23697200
C	2.65450300	3.91626400	-3.57678800
H	3.17286000	3.09205400	-4.07184700
C	3.55324800	5.14005100	-3.66210300
O	4.01995000	5.54375100	-4.69327100
O	3.75521000	5.72277300	-2.46964900
H	4.33347800	6.48872500	-2.63210000
H	1.73462900	4.13717600	-4.12486600
H	3.19216100	-3.42641800	-3.86478800
H	-4.60423500	-1.03435400	-4.20807500
C	-0.04297400	0.01538100	0.21082100
H	-0.62969900	-0.86727800	0.47855800
H	0.63779300	0.26122800	1.03056300
H	0.53485500	-0.18843800	-0.69433100
H	-0.71687800	0.85706500	0.03061900

Sum of electronic and zero-point Energies= -2836.860122

Sum of electronic and thermal Energies= -2836.810837

Sum of electronic and thermal Enthalpies= -2836.809892

Sum of electronic and thermal Free Energies= -2836.950178

Basket [**1**–C_2H_6]

C	0.90676400	2.10808500	3.27332400
C	0.76365400	0.86593600	3.82573000
C	-0.52466500	0.27181200	3.92394300
C	-1.61991200	0.94865100	3.45887000
C	-1.46720400	2.23132900	2.85745100
C	-0.22488400	2.79927100	2.75820100
C	1.75892900	-0.18376300	4.31085900
H	2.75536900	0.17022600	4.57673400
C	-0.30385700	-1.13557800	4.48115900
H	-1.17428100	-1.63919800	4.90250000
C	0.90371200	-0.85761000	5.41775200
H	0.65829700	-0.17475000	6.23542100
H	1.35640400	-1.77443400	5.80522500
C	1.69319700	-1.26951600	3.23965500
C	0.41979200	-1.87024100	3.35447900
C	2.12218900	2.97190400	2.95536800
H	3.03083200	2.76468300	3.52142600
C	0.31748100	4.07381300	2.10620400
H	-0.40441200	4.86589100	1.90441400
C	1.48171800	4.38099000	3.08935700
H	2.13802400	5.17889900	2.73094000
H	1.13413800	4.59481800	4.10353200
C	1.13305700	3.58319300	0.90743900
C	2.24351600	2.89230100	1.44064300
C	-3.10622800	0.61361700	3.38244100
H	-3.46076200	-0.17785700	4.04364100
C	-2.86425100	2.66335400	2.41602400
H	-3.00018600	3.72425500	2.20418800
C	-3.69134300	2.04253200	3.57956700
H	-3.44105800	2.47193700	4.55350800
H	-4.76990600	2.08696400	3.40464000
C	-3.41473200	0.43274900	1.89973900
C	-3.26726500	1.70332300	1.30067900
C	1.82380000	2.97269800	-1.26001900
C	2.90522500	2.28313400	-0.72757400
C	2.13373100	-2.59765300	1.35094100
C	0.88939700	-3.20244800	1.47356700
C	-0.01028800	-2.85401700	2.47764400
C	2.57633800	-1.61249200	2.22797100
C	-3.77444600	-0.68751100	1.16812000
C	-3.48076400	1.90407300	-0.05392200
C	3.15039100	2.21933500	0.63925800

C	0.90107400	3.64335900	-0.45905000
H	-0.98915700	-3.31974200	2.54360500
H	3.55067500	-1.14879700	2.10464300
H	-3.89826700	-1.67167200	1.60992500
H	-3.38039500	2.87407100	-0.53162400
H	0.05051300	4.15910000	-0.89539800
H	4.00231800	1.67348000	1.03491800
C	0.73678500	-4.18776800	0.35958300
C	2.81426500	-3.16542100	0.14938100
N	1.89722600	-4.05891500	-0.41306200
O	-0.17256300	-4.94469800	0.12842200
O	3.91240700	-2.93619300	-0.29182900
C	3.66656400	1.65857100	-1.84869300
C	1.85950300	2.81225500	-2.74663800
N	2.94458700	1.96523900	-3.00641500
O	4.68609500	1.01581000	-1.81659900
O	1.13079500	3.28121300	-3.58469200
C	3.43173900	1.67413000	-4.32496600
H	3.89619500	0.68460800	-4.32927700
C	4.46419700	2.66604200	-4.83836300
O	5.01494500	2.55251300	-5.90036500
O	4.68724900	3.67688000	-3.98324600
H	5.35739900	4.24653000	-4.39994800
C	2.22075000	-4.91155800	-1.52116900
H	1.29000900	-5.34895900	-1.89343400
C	3.16956900	-6.04719800	-1.17302900
O	3.68030700	-6.75489200	-1.99893700
O	3.35334200	-6.18554500	0.14950200
H	3.96698600	-6.93199200	0.26581200
C	-3.85962500	0.77671100	-0.77827400
C	-3.99984200	-0.47326800	-0.18860100
C	-4.20682400	0.65045900	-2.22585500
C	-4.44014200	-1.44098000	-1.23794800
O	-4.26600100	1.50048700	-3.07866100
O	-4.71692300	-2.60932300	-1.13091300
N	-4.47861700	-0.70742200	-2.42957900
C	-5.01626400	-1.21905800	-3.65816800
H	-4.47240500	-0.79886600	-4.50726300
C	-6.49198900	-0.91504100	-3.86425400
O	-7.07793300	-1.15505200	-4.88574900
O	-7.06943700	-0.37009800	-2.78194700
H	-8.00212500	-0.21902700	-3.01567800
H	-4.89333000	-2.30570800	-3.66109400
H	2.58958700	1.67374400	-5.02178700
H	2.68534800	-4.33187600	-2.32215000
C	0.83014000	-0.48595400	-1.01477700
H	1.89567700	-0.47485600	-0.75537600
H	0.70656200	0.08636700	-1.94167700
H	0.55232600	-1.52325400	-1.23415400
C	-0.02420300	0.08978000	0.11130000
H	-1.08801500	0.07849600	-0.14984600
H	0.09510600	-0.47892400	1.03898300
H	0.24938000	1.12670000	0.32607000

Sum of electronic and zero-point Energies= -2876.124669

Sum of electronic and thermal Energies= -2876.075972

Sum of electronic and thermal Enthalpies= -2876.075028

Sum of electronic and thermal Free Energies= -2876.212236

Basket [**1**–C_3H_8]

0 1

C	1.09004800	1.90006100	3.38453600
C	0.01888700	1.21139600	3.88407900
C	-1.30278900	1.60547700	3.53640000

C	-1.50183200	2.68395600	2.71745300
C	-0.38604200	3.39649200	2.19370800
C	0.88680200	3.01580900	2.52469800
C	-0.11522700	-0.06248400	4.71717900
H	0.74708900	-0.34384900	5.32232400
C	-2.23085300	0.55351100	4.13909300
H	-3.28566800	0.81816400	4.22061000
C	-1.45152600	0.24488400	5.44728500
H	-1.38281900	1.11044400	6.11147700
H	-1.84904200	-0.62137300	5.98333600
C	-0.60965400	-1.10702000	3.72211100
C	-1.91641000	-0.71865700	3.35316500
C	2.59846500	1.69380400	3.46857700
H	2.96153800	1.07424700	4.28924900
C	2.27847900	3.49252400	2.10683900
H	2.34733700	4.50263200	1.70168900
C	3.05603900	3.17883200	3.41695300
H	4.13813300	3.28655400	3.30184900
H	2.69979000	3.76090100	4.27119700
C	2.83513500	2.37843400	1.22613500
C	3.01577000	1.25770500	2.06619600
C	-2.74494600	3.30235900	2.07941300
H	-3.69789000	3.10103800	2.56966700
C	-0.95915200	4.43039800	1.22643300
H	-0.29983000	5.24974000	0.93836500
C	-2.27395900	4.77923100	1.97683700
H	-2.09433600	5.23533200	2.95396600
H	-2.95044700	5.39894600	1.38159000
C	-2.64855400	2.90708400	0.61024000
C	-1.53569700	3.59786700	0.08225200
C	3.57382800	1.10836800	-0.60970600
C	3.72715700	-0.00094000	0.21194500
C	-0.70000200	-2.86394400	2.16321300
C	-1.98408100	-2.48105600	1.79850300
C	-2.63336600	-1.39499000	2.37861500
C	0.02900100	-2.18991000	3.13887800
C	-3.37168800	1.99150900	-0.13795900
C	-1.09847200	3.39297200	-1.21702900
C	3.45149700	0.03682600	1.57591200
C	3.11501000	2.33251100	-0.13056300
H	-3.63282300	-1.10547400	2.06726300
H	1.03838800	-2.49495000	3.39982500
H	-4.22492000	1.44623700	0.25501900
H	-0.23892100	3.90219000	-1.64295900
H	2.99276400	3.18508000	-0.79217800
H	3.58676000	-0.84082900	2.20134000
C	-2.44592900	-3.37978700	0.69659300
C	-0.29641900	-4.02079400	1.30888200
N	-1.36191400	-4.22325600	0.42668700
O	-3.50358900	-3.39729800	0.11890400
O	0.72155700	-4.66726100	1.32119600
C	4.23091200	-1.13632300	-0.61915200
C	3.98227100	0.72345500	-1.99402000
N	4.30540000	-0.63589200	-1.92517200
O	4.51968200	-2.25745800	-0.28409400
O	4.04833400	1.39540400	-2.99299000
C	4.85589800	-1.36034900	-3.03617500
H	4.94150400	-2.40879000	-2.73333800
C	6.22965100	-0.87176900	-3.46533600
O	6.72506600	-1.13999100	-4.52662900
O	6.84051400	-0.14325900	-2.51706300
H	7.70406900	0.11592700	-2.88367100
C	-1.39821400	-5.30241400	-0.51872800
H	-2.22735500	-5.11683400	-1.20816600

C	-1.60163900	-6.67388000	0.10508500
O	-1.46731000	-7.70051700	-0.50484100
O	-1.97194300	-6.61133700	1.39380200
H	-2.07693400	-7.53125800	1.69421600
C	-1.83260200	2.47444000	-1.96256400
C	-2.92901700	1.79824000	-1.44304900
C	-1.63237800	2.02860100	-3.37520700
C	-3.46531300	0.89351100	-2.50363300
O	-0.82446000	2.40513900	-4.18687900
O	-4.43184600	0.17363800	-2.48433400
N	-2.60091600	1.04191100	-3.59501200
C	-2.86356200	0.44733300	-4.87516400
H	-1.96826400	0.56410500	-5.49286400
C	-4.03455700	1.07196900	-5.61720000
O	-4.51802900	0.59450800	-6.60835800
O	-4.44827200	2.22178000	-5.06142700
H	-5.19030600	2.53996100	-5.60502400
H	-3.07873000	-0.61739500	-4.76097200
H	4.20009200	-1.29558100	-3.90721500
H	-0.46594700	-5.33746900	-1.08769300
C	-0.39322400	-0.79370600	-0.84595800
H	-0.66310000	-0.27562300	-1.77582700
H	-1.28637000	-1.35837600	-0.55058700
C	-0.05066900	0.22886900	0.23375300
H	-0.90954400	0.85914600	0.48569600
H	0.27610300	-0.27138100	1.15382700
H	0.76539000	0.88439600	-0.09345300
C	0.76466500	-1.75094900	-1.11974600
H	1.12296200	-2.22238800	-0.19566400
H	0.48290200	-2.54599600	-1.81792400
H	1.61235000	-1.21036000	-1.55740800

Sum of electronic and zero-point Energies= -2915.393348

Sum of electronic and thermal Energies= -2915.343420

Sum of electronic and thermal Enthalpies= -2915.342476

Sum of electronic and thermal Free Energies= -2915.483434

Basket [**2**]

C	1.40023100	-0.87964600	3.41944400
C	0.19225200	-1.51942100	3.48124900
C	-1.01032500	-0.76277700	3.56902600
C	-0.95842100	0.60427100	3.59034000
C	0.29781400	1.27007400	3.52168300
C	1.45366200	0.54265700	3.43834900
C	-0.22710600	-2.98753200	3.46341000
H	0.54905700	-3.71863200	3.69173200
C	-2.15192800	-1.77603500	3.60512900
H	-3.11509400	-1.41162300	3.96333500
C	-1.45403900	-2.90606600	4.41624100
H	-1.18401500	-2.59565000	5.42915900
H	-2.03545100	-3.83187200	4.43897000
C	-0.96369600	-3.18720400	2.14223500
C	-2.15671100	-2.43700600	2.22995200
C	2.84546900	-1.36018600	3.31340800
H	3.03325400	-2.40112600	3.57842200
C	2.93082100	0.91679900	3.34108500
H	3.19519000	1.93426800	3.63068200
C	3.53617900	-0.25594500	4.16509900
H	4.62738600	-0.29670200	4.10649900
H	3.20591500	-0.25618400	5.20728100
C	3.37471200	0.48318600	1.94725100
C	3.32248500	-0.92760500	1.93034300
C	-2.01957700	1.69963300	3.66465600
H	-3.00698000	1.39711600	4.01472800

C	-0.00853300	2.76550200	3.55305200
H	0.82156500	3.42704500	3.80256100
C	-1.23577700	2.74497700	4.50935600
H	-0.98699500	2.38029000	5.50956700
H	-1.74457100	3.71125100	4.56686700
C	-1.97744200	2.40465200	2.31267700
C	-0.73178800	3.06562600	2.24336400
C	4.10196100	0.47144400	-0.28829900
C	4.05149800	-0.91590000	-0.30422700
C	-1.55745200	-3.85906300	-0.03081600
C	-2.73084800	-3.12166600	0.05541700
C	-3.06633400	-2.38213200	1.18578700
C	-0.63310500	-3.91175800	1.00795200
C	-2.89271000	2.45266400	1.27318600
C	-0.35329000	3.80298400	1.13243400
C	3.65349200	-1.66084400	0.80179300
C	3.75942000	1.21688800	0.83608900
H	-3.99047900	-1.81365000	1.23210300
H	0.27716700	-4.49788900	0.92337300
H	-3.85655500	1.95338000	1.30789700
H	0.59809100	4.32169500	1.05992200
H	3.80798900	2.30173800	0.82880000
H	3.62335800	-2.74584600	0.76841300
C	-3.49086600	-3.29915300	-1.21955700
C	-1.53018900	-4.53484600	-1.36280800
N	-2.69175100	-4.12218700	-2.02035500
O	-4.56474400	-2.84922300	-1.53381200
O	-0.71118300	-5.29563300	-1.81920900
C	4.49972000	-1.38626500	-1.65012200
C	4.58492900	0.93443200	-1.62402100
N	4.76769200	-0.22487800	-2.38285800
O	4.62052200	-2.51418900	-2.05973400
O	4.80027600	2.05650200	-2.01390800
C	5.28837600	-0.22073300	-3.73303700
H	5.50397800	-1.27298400	-3.95866500
C	6.61982900	0.52178100	-3.80377700
O	7.01802000	1.09633100	-4.78177100
O	7.33130600	0.40920000	-2.66945100
H	8.15778600	0.90162900	-2.81534900
C	-3.07734700	-4.60062800	-3.33096700
H	-4.11429700	-4.26574600	-3.46336500
C	-3.10179300	-6.12608500	-3.36800900
O	-2.87927900	-6.77933300	-4.35233900
O	-3.46336200	-6.66120400	-2.18949600
H	-3.45879400	-7.62611600	-2.31486600
C	-1.28435300	3.85660100	0.09966000
C	-2.50843000	3.20470900	0.16687300
C	-1.20933100	4.57935400	-1.20664200
C	-3.25632800	3.48877900	-1.09478000
O	-0.32859400	5.28171500	-1.63724200
O	-4.36615200	3.14371200	-1.42130700
N	-2.40459700	4.28037700	-1.86945300
C	-2.77879100	4.83354700	-3.15364500
H	-1.99513200	5.56556900	-3.38827000
C	-4.08693900	5.61310300	-3.05127000
O	-4.86588700	5.74317200	-3.95763900
O	-4.24390600	6.19541300	-1.85047200
H	-5.09324600	6.66891600	-1.88548800
C	-2.86297100	3.77478500	-4.24679800
H	-3.60858800	3.02229700	-3.97961000
H	-3.16176300	4.24074700	-5.18707300
H	-1.88944200	3.29559100	-4.37074300
C	4.29734300	0.34643500	-4.74303900
H	4.05785900	1.38151900	-4.48913600

H	4.73751400	0.32652200	-5.74124000
H	3.38350200	-0.25160100	-4.73697900
C	-2.19319100	-4.04589100	-4.44167200
H	-2.25331000	-2.95536700	-4.44900500
H	-1.15709100	-4.35316100	-4.28190800
H	-2.52599700	-4.43432200	-5.40543400

Sum of electronic and zero-point Energies= -2914.223168

Sum of electronic and thermal Energies= -2914.173508

Sum of electronic and thermal Enthalpies= -2914.172564

Sum of electronic and thermal Free Energies= -2914.312563

Basket [**2**–CH_4]

C	1.40453800	-0.89577100	3.54457500
C	0.19213800	-1.52684000	3.60426800
C	-1.00441100	-0.76256500	3.69910000
C	-0.94269800	0.60416800	3.72501200
C	0.31803900	1.26147900	3.65653300
C	1.46879000	0.52591400	3.57055700
C	-0.24076700	-2.98837900	3.50945700
H	0.52221300	-3.73886700	3.71843600
C	-2.15640400	-1.76437800	3.66499500
H	-3.12476600	-1.40756700	4.01668100
C	-1.49052900	-2.94142300	4.43273100
H	-1.24310600	-2.68583100	5.46650100
H	-2.08130100	-3.86071300	4.39408700
C	-0.93925400	-3.10237700	2.15702000
C	-2.12693200	-2.34429900	2.25398200
C	2.83875600	-1.38468300	3.35485700
H	3.03546100	-2.42916700	3.59845300
C	2.94130900	0.89108100	3.39551800
H	3.23009800	1.90447500	3.67601600
C	3.58835100	-0.29242600	4.16873400
H	4.67335800	-0.33918900	4.04112700
H	3.32439100	-0.29964400	5.22968800
C	3.28310000	0.46718000	1.97004200
C	3.21811900	-0.94329600	1.94453700
C	-2.00019700	1.70514000	3.72446500
H	-2.99795800	1.42460400	4.06352100
C	0.01729500	2.75774400	3.60851400
H	0.84321500	3.43021600	3.84226900
C	-1.23490700	2.79277900	4.52930900
H	-1.01440100	2.48420200	5.55469400
H	-1.74133200	3.76196200	4.51907300
C	-1.91470600	2.32409100	2.33217400
C	-0.66406400	2.97578900	2.25995100
C	3.78332300	0.47394200	-0.32662900
C	3.71873100	-0.91268800	-0.35168200
C	-1.44020900	-3.58006300	-0.08973800
C	-2.60752400	-2.83441300	0.00611500
C	-2.98833800	-2.19016800	1.17952100
C	-0.56671500	-3.73699100	0.98261500
C	-2.78385500	2.28151500	1.25341600
C	-0.23207100	3.60850900	1.10501900
C	3.43062800	-1.66700700	0.78205200
C	3.56460800	1.20987900	0.83432200
H	-3.90549800	-1.61044100	1.23061600
H	0.34282300	-4.32321000	0.88742900
H	-3.74954100	1.78526900	1.28785800
H	0.72679200	4.11271900	1.02595200
H	3.62031200	2.29459000	0.83213900
H	3.38514800	-2.75144900	0.73980100
C	-3.30350900	-2.87975000	-1.31549000
C	-1.35423100	-4.13152200	-1.47607900

N	-2.47196200	-3.63313200	-2.15127500
O	-4.35633100	-2.38719500	-1.63704600
O	-0.52586900	-4.86565900	-1.95797400
C	4.02179100	-1.37140100	-1.74182700
C	4.13340300	0.94780500	-1.69922800
N	4.21482100	-0.20309800	-2.48781900
O	4.09714600	-2.49551200	-2.17165000
O	4.33154800	2.07121300	-2.09429100
C	4.61376200	-0.18562300	-3.87898700
H	4.78482400	-1.23805500	-4.14015000
C	5.95107800	0.52920500	-4.05306800
O	6.27480900	1.11949500	-5.04910800
O	6.75749600	0.37121200	-2.98955200
H	7.58080000	0.84667000	-3.19694700
C	-2.80300000	-3.98422200	-3.51560000
H	-3.81714900	-3.59386700	-3.67119800
C	-2.88869300	-5.49810100	-3.68979900
O	-2.68604800	-6.06773500	-4.72930500
O	-3.28211600	-6.12322300	-2.56728800
H	-3.32349200	-7.07117500	-2.78380900
C	-1.11424500	3.56559600	0.02932300
C	-2.34444500	2.92627800	0.10069900
C	-0.97075600	4.15562200	-1.33651600
C	-3.03019700	3.08880800	-1.21682600
O	-0.06561400	4.81065300	-1.79013700
O	-4.12796200	2.72177400	-1.55927300
N	-2.13400100	3.79367600	-2.02492000
C	-2.43970300	4.21487100	-3.37542800
H	-1.63417200	4.90968300	-3.64639200
C	-3.73861800	5.01475700	-3.41791000
O	-4.47267900	5.05540500	-4.36917800
O	-3.94154200	5.72381700	-2.29450700
H	-4.77828800	6.20390800	-2.42245800
C	0.04392200	-0.06351500	0.22440000
H	0.50747000	-1.02000500	0.47867200
H	0.58493700	0.74470100	0.72232300
H	0.08160900	0.08486800	-0.85720000
H	-0.99666100	-0.06179900	0.55887900
C	-2.48934800	3.04875400	-4.35600600
H	-3.27020600	2.34533200	-4.05817300
H	-2.71759100	3.41817600	-5.35705600
H	-1.52369600	2.53825300	-4.36884800
C	3.55164900	0.42364900	-4.78667000
H	3.35628200	1.45671100	-4.48957800
H	3.90418600	0.41994700	-5.81927300
H	2.62944100	-0.15712600	-4.71519200
C	-1.83977300	-3.37725700	-4.53003500
H	-1.85873200	-2.28799900	-4.44980900
H	-0.82588400	-3.73897100	-4.34355600
H	-2.13520800	-3.67298300	-5.53787200

Sum of electronic and zero-point Energies= -2954.668772

Sum of electronic and thermal Energies= -2954.615903

Sum of electronic and thermal Enthalpies= -2954.614958

Sum of electronic and thermal Free Energies= -2954.760640

Basket [**2**−C_2H_6]

C	1.88995400	-2.41512000	-2.94552500
C	1.85733000	-1.22115300	-3.61331200
C	0.62162900	-0.71313500	-4.10258700
C	-0.53523700	-1.41212300	-3.89019700
C	-0.50237300	-2.65155700	-3.19140200
C	0.68889800	-3.14965900	-2.73800100
C	2.90620700	-0.15424400	-3.91773800
H	3.94995800	-0.46748400	-3.87919000

C	0.92984100	0.65342100	-4.71260600
H	0.18409500	1.06370200	-5.39418700
C	2.35127200	0.36966300	-5.27176600
H	2.35420300	-0.39419400	-6.05393600
H	2.85901600	1.27505200	-5.61559100
C	2.52448200	1.01984800	-3.02094100
C	1.30325600	1.52672000	-3.51817100
C	2.99188300	-3.18632300	-2.22282000
H	4.01912700	-2.94195200	-2.49485800
C	1.07289400	-4.37147200	-1.90353400
H	0.36296100	-5.19925400	-1.89367700
C	2.49381700	-4.63576100	-2.47533700
H	3.04883400	-5.38144500	-1.89934400
H	2.48167100	-4.89983100	-3.53599800
C	1.45647700	-3.79788800	-0.54310900
C	2.64141300	-3.05542100	-0.74338100
C	-2.00342100	-1.12960700	-4.19444600
H	-2.20661500	-0.38825700	-4.96790700
C	-1.95304800	-3.11131000	-3.07076800
H	-2.11415300	-4.16253900	-2.82953000
C	-2.49488900	-2.58620200	-4.43146800
H	-2.01226300	-3.06129100	-5.28996900
H	-3.58288000	-2.65957600	-4.51192300
C	-2.65301900	-0.87376900	-2.83796900
C	-2.62182200	-2.10160600	-2.14072700
C	1.40958900	-3.09548700	1.69970900
C	2.56994700	-2.35986700	1.49997300
C	2.43135200	2.56907100	-1.25692800
C	1.23141400	3.06831600	-1.74415400
C	0.62724300	2.56215700	-2.89201500
C	3.11514800	1.52673000	-1.87494800
C	-3.18703200	0.27572400	-2.27739300
C	-3.12521000	-2.22847700	-0.85538700
C	3.22276400	-2.31302100	0.27217500
C	0.81238600	-3.83617900	0.68345800
H	-0.31717000	2.95804500	-3.25384200
H	4.04680000	1.14542300	-1.46669000
H	-3.22194200	1.22878600	-2.79711200
H	-3.11362900	-3.16259600	-0.30162200
H	-0.10610800	-4.38958000	0.85587500
H	4.12381200	-1.72162300	0.13593500
C	0.77114500	4.15439200	-0.82566800
C	2.78440600	3.32659500	-0.01977800
N	1.71367800	4.19515900	0.21042500
O	-0.19716700	4.86712900	-0.91549900
O	3.77833400	3.25360700	0.66129900
C	2.90386100	-1.65457400	2.77446600
C	0.97426000	-2.90120700	3.11529800
N	1.88965800	-2.00476100	3.67250700
O	3.83129800	-0.92269400	3.01648300
O	0.04263200	-3.39340800	3.70478000
C	1.83370600	-1.56360000	5.04971000
H	2.78665300	-1.04753900	5.22427300
C	1.80132100	-2.75438000	6.00342700
O	1.27288600	-2.73724000	7.08320600
O	2.48865800	-3.80788700	5.53115000
H	2.42219500	-4.50359800	6.20823300
C	1.72191900	5.20525800	1.24689900
H	0.81285800	5.79590000	1.07439000
C	2.89729800	6.16257600	1.06871900
O	3.38436400	6.80407600	1.96149500
O	3.29369800	6.25780300	-0.21234300
H	4.02633100	6.89804300	-0.22599500
C	-3.67691700	-1.07330300	-0.30828100

C	-3.70518700	0.13451000	-0.99308800
C	-4.33086200	-0.87329600	1.02101300
C	-4.37677500	1.14706600	-0.12353500
O	-4.53015700	-1.67670800	1.89796600
O	-4.63203100	2.30465500	-0.35280900
N	-4.68884100	0.47865000	1.06302900
C	-5.40451400	1.09375300	2.16026800
H	-5.67126200	0.26419800	2.82786200
C	-6.71829400	1.70712600	1.68308400
O	-7.25195600	2.64647700	2.21098400
O	-7.25082600	1.03925600	0.64602000
H	-8.08193800	1.49466000	0.42507200
C	0.85160200	0.48902600	0.92698200
H	1.94423900	0.49261800	0.83762300
H	0.59701400	-0.02866500	1.85964800
H	0.52397100	1.53018800	1.03195000
C	0.19084400	-0.18217800	-0.27529500
H	-0.90005000	-0.18415100	-0.17682800
H	0.43808500	0.33599200	-1.20728400
H	0.51573700	-1.22277700	-0.38076100
C	-4.56310900	2.12488800	2.90382200
H	-4.25718300	2.91973700	2.21962900
H	-5.15045100	2.56738700	3.70986400
H	-3.67636500	1.64322400	3.32205000
C	0.66275200	-0.62339300	5.31194600
H	-0.27864300	-1.13094400	5.08777600
H	0.65492200	-0.32620700	6.36185900
H	0.75701600	0.26526900	4.68307700
C	1.71153500	4.61181600	2.65219300
H	0.82515400	3.98611000	2.78166000
H	2.60707700	4.00768400	2.81245300
H	1.69678700	5.41753800	3.38823300

Sum of electronic and zero-point Energies= -2993.934031

Sum of electronic and thermal Energies= -2993.879635

Sum of electronic and thermal Enthalpies= -2993.878691

Sum of electronic and thermal Free Energies= -2994.027667

Basket [**2**−C_3H_8]

C	0.12207900	-3.28049700	-2.68162000
C	-0.69988900	-2.46087200	-3.40500000
C	-2.04542500	-2.25983800	-2.98974700
C	-2.52833400	-2.91683700	-1.89035200
C	-1.67150400	-3.77021800	-1.13923200
C	-0.36972700	-3.94546200	-1.52416900
C	-0.47319900	-1.53861800	-4.60142000
H	0.37876200	-1.76940600	-5.24192200
C	-2.61652600	-1.18759400	-3.91367800
H	-3.70179600	-1.08562200	-3.93545000
C	-1.89260900	-1.57864200	-5.23197000
H	-2.17163900	-2.57473500	-5.58598200
H	-2.02433700	-0.83720300	-6.02463200
C	-0.50644400	-0.13647000	-4.00575400
C	-1.83095100	0.07674300	-3.56350200
C	1.60595300	-3.61972300	-2.77202300
H	2.09069700	-3.44277900	-3.73242500
C	0.81908300	-4.69467100	-0.92343000
H	0.58747900	-5.49122000	-0.21557300
C	1.56396900	-5.07747900	-2.23356800
H	2.55885000	-5.49181800	-2.04954000
H	0.98040200	-5.74614200	-2.87214800
C	1.76128700	-3.60424200	-0.42099500
C	2.23671500	-2.92807500	-1.56623900
C	-3.86082800	-2.88106700	-1.14322700
H	-4.72674700	-2.53185400	-1.70628400

C	-2.48331000	-4.23211000	0.06788200
H	-2.10664500	-5.10168100	0.60702100
C	-3.88540800	-4.33488100	-0.59452400
H	-3.92369500	-5.08633400	-1.38757200
H	-4.68639200	-4.49939300	0.13139600
C	-3.55467500	-2.13482300	0.15036000
C	-2.69049500	-2.96629600	0.89604100
C	2.98982000	-2.13483200	0.94235500
C	3.43816900	-1.45594500	-0.18273900
C	0.11667100	1.95440800	-3.13343500
C	-1.18189900	2.16044300	-2.68874300
C	-2.19791100	1.22896800	-2.88647400
C	0.49836800	0.79632000	-3.80495700
C	-3.91032800	-0.86641200	0.58175500
C	-2.13723800	-2.55563200	2.09876700
C	3.07538600	-1.82867000	-1.47359400
C	2.12987800	-3.22654100	0.86066600
H	-3.20614400	1.41313200	-2.52692700
H	1.52136800	0.64889800	-4.13900300
H	-4.57173700	-0.21189600	0.02159100
H	-1.46381500	-3.17300500	2.68586200
H	1.78409600	-3.73957600	1.75346900
H	3.44641800	-1.28839200	-2.33998200
C	-1.23653800	3.49039100	-2.00855700
C	0.93003900	3.15199500	-2.76671900
N	0.07368600	3.98461000	-2.04021900
O	-2.18410800	4.05352300	-1.51992000
O	2.08055900	3.40346300	-3.03298400
C	4.33885800	-0.34963800	0.26377200
C	3.59690000	-1.49131800	2.14619400
N	4.35866700	-0.42473100	1.66110400
O	4.93898900	0.45729300	-0.40136600
O	3.49555800	-1.79511000	3.31014100
C	5.14805800	0.44232600	2.50932300
H	5.78195100	1.01606300	1.82087200
C	6.08926700	-0.36864400	3.39488800
O	6.45588500	-0.01911500	4.48515400
O	6.52055900	-1.48948400	2.79226000
H	7.11716100	-1.92620200	3.42496000
C	0.43489100	5.32490700	-1.62792500
H	-0.49890000	5.76892100	-1.25878900
C	0.86541300	6.16725500	-2.82684700
O	1.61484700	7.10502000	-2.75847500
O	0.26000000	5.78486400	-3.96490700
H	0.57476900	6.38863300	-4.65996900
C	-2.49853600	-1.28051700	2.52276200
C	-3.35466900	-0.46640300	1.79311200
C	-2.08806800	-0.54260300	3.75619300
C	-3.52031800	0.81885900	2.53601500
O	-1.38460600	-0.91139000	4.66361300
O	-4.21482400	1.77033000	2.27349700
N	-2.69661600	0.71390900	3.66048500
C	-2.61798900	1.73266400	4.68570500
H	-2.06658900	1.26458000	5.51149800
C	-4.00459600	2.07120200	5.22625600
O	-4.30709700	3.14179600	5.68216400
O	-4.83647100	1.01619900	5.19725500
H	-5.68122300	1.32337200	5.57005200
C	-0.19461300	0.93329500	0.48609900
H	-0.58703600	0.80893100	1.50427900
H	-0.85774900	1.65832500	-0.00292500
C	-0.25019400	-0.39950300	-0.25514600
H	-1.27817100	-0.75653100	-0.37549900
H	0.19032800	-0.30486700	-1.25547100

H	0.31441700	-1.17044800	0.28305000
C	1.22520200	1.48954300	0.55407800
H	1.65294200	1.61372000	-0.44922700
H	1.26110500	2.46000800	1.05932000
H	1.87871500	0.80235100	1.10575700
C	-1.89776700	2.98825100	4.20734900
H	-2.42843600	3.42065000	3.35582300
H	-1.86993000	3.72561200	5.01143100
H	-0.87745200	2.73486500	3.90946000
C	4.28605300	1.38011000	3.34593300
H	3.62322800	0.79831300	3.99122700
H	4.92246400	2.00513800	3.97417500
H	3.68891200	2.01418000	2.68651800
C	1.50008700	5.34727200	-0.53760200
H	1.12553800	4.83751300	0.35292700
H	2.40737800	4.84939700	-0.88745700
H	1.74403300	6.38159100	-0.28886900

Sum of electronic and zero-point Energies= -3033.201856

Sum of electronic and thermal Energies= -3033.146314

Sum of electronic and thermal Enthalpies= -3033.145369

Sum of electronic and thermal Free Energies= -3033.297025

Basket [**3**]

C	0.90939400	-0.57518000	4.39372300
C	-0.41859200	-0.25107700	4.46055600
C	-0.83493300	1.09389600	4.25115000
C	0.09279200	2.06391800	3.98419200
C	1.47486200	1.72948900	3.92897700
C	1.87415600	0.43615400	4.12625600
C	-1.69108300	-1.06072300	4.69751900
H	-1.56536500	-2.04002400	5.16014100
C	-2.35765700	1.09242000	4.36333000
H	-2.83444700	2.05970700	4.52453900
C	-2.52280400	0.00643600	5.46546800
H	-2.06677600	0.29532200	6.41625900
H	-3.56423700	-0.29291200	5.61281500
C	-2.44317000	-1.04120700	3.37004500
C	-2.85806600	0.29311700	3.16388300
C	1.68618500	-1.88581800	4.50835300
H	1.17268900	-2.71659900	4.99315800
C	3.22913300	-0.26434700	4.08123300
H	4.11002800	0.37101600	4.17834400
C	2.98699700	-1.34742300	5.17013500
H	3.78367900	-2.09547100	5.20940900
H	2.81175600	-0.91920100	6.16063200
C	3.17846200	-1.15146800	2.84098300
C	2.22342300	-2.15732700	3.10548500
C	0.00206200	3.55430700	3.66384000
H	-0.92720900	4.05649000	3.93450300
C	2.21569900	3.01969900	3.58724300
H	3.28672100	3.03510800	3.79110800
C	1.31454900	4.03460200	4.34652300
H	1.31281600	3.87288600	5.42779400
H	1.55818000	5.07461900	4.11279000
C	0.42988500	3.68114400	2.20339700
C	1.80277300	3.35258500	2.15753000
C	3.52372500	-2.05464100	0.69920400
C	2.58692700	-3.04519100	0.95954300
C	-3.43597600	-1.65233800	1.32985100
C	-3.84483900	-0.34444000	1.12978600
C	-3.56470600	0.67526400	2.03504800
C	-2.71548200	-2.04494800	2.45438800
C	-0.28302300	4.01099200	1.06151400

C	2.51722400	3.34386000	0.97048400
C	1.90108700	-3.12579200	2.16807900
C	3.84558700	-1.07089300	1.62888900
H	-3.89602400	1.69403500	1.85718300
H	-2.40542500	-3.07650900	2.59264000
H	-1.33832300	4.26694500	1.07303800
H	3.57305000	3.09550900	0.91436900
H	4.57841200	-0.30112300	1.40522300
H	1.16836000	-3.90661900	2.34829500
C	-4.59152900	-0.29768600	-0.15707500
C	-3.90151100	-2.48586300	0.17669400
N	-4.57650000	-1.60267900	-0.67855200
O	-5.12682500	0.63928200	-0.69705900
O	-3.71832700	-3.66907500	0.02386300
C	2.49309200	-3.92460200	-0.24451200
C	4.05508500	-2.26306000	-0.68175500
N	3.38356100	-3.38449900	-1.17973800
O	1.81109200	-4.90384700	-0.42158600
O	4.88727300	-1.62456800	-1.27844600
C	3.58502500	-3.97244500	-2.49271600
H	3.32755300	-5.03364800	-2.36680600
C	5.06902500	-3.94635000	-2.85234300
O	5.52554200	-3.67545600	-3.93150000
O	5.82640700	-4.35607400	-1.81955800
H	6.75014900	-4.30142400	-2.12063300
C	-5.25392400	-1.82932200	-1.94967000
H	-4.83738700	-1.11267200	-2.66562100
C	-6.73251600	-1.47199600	-1.84430000
O	-7.41489600	-1.17763700	-2.79140500
O	-7.21875400	-1.59254700	-0.59718500
H	-8.16253700	-1.36073700	-0.65230300
C	1.79496000	3.68903300	-0.16793700
C	0.44536800	4.00906600	-0.12475700
C	2.25738300	3.80671900	-1.58295300
C	-0.00303500	4.33460900	-1.51259500
O	3.36571300	3.65484300	-2.03441500
O	-1.09023900	4.69385700	-1.89178100
N	1.12160500	4.15130300	-2.32702800
C	1.17560700	4.43295700	-3.74977400
H	2.23650000	4.63914400	-3.95142900
C	0.43644000	5.72678900	-4.07635800
O	-0.20339900	5.91339300	-5.07742800
O	0.66362600	6.68045300	-3.15683900
H	0.16553300	7.46442600	-3.44685300
C	0.73367600	3.26048200	-4.63726400
H	0.80667500	3.63658700	-5.66456600
C	2.64776300	-3.37561600	-3.55645000
H	1.64702400	-3.46933800	-3.11277800
C	-5.10310800	-3.25812600	-2.52721000
H	-4.07026000	-3.56287600	-2.33904400
C	1.69197800	2.08195800	-4.46503600
H	2.73262300	2.36666900	-4.64778100
H	1.63207200	1.67816300	-3.44759100
H	1.42702500	1.27605300	-5.15615700
C	-0.71091200	2.83274600	-4.38194200
H	-1.00148900	2.06760000	-5.10863300
H	-0.81852600	2.39736400	-3.38240400
H	-1.40310000	3.67310700	-4.46586300
C	2.66627200	-4.20536300	-4.84230100
H	1.87994300	-3.85625000	-5.51833300
H	3.62683400	-4.11165500	-5.35278700
H	2.48130200	-5.26534000	-4.63559400
C	2.91867300	-1.89678300	-3.83460600
H	2.19330000	-1.52215900	-4.56381900

H	2.82865900	-1.28745100	-2.93084500
H	3.92275900	-1.75458600	-4.24215900
C	-5.33934100	-3.22515200	-4.03870700
H	-5.23190100	-4.23247400	-4.45210200
H	-6.34431900	-2.86174000	-4.27153800
H	-4.61779800	-2.57301500	-4.54111200
C	-6.04096100	-4.26311600	-1.85542700
H	-7.08331200	-4.05844800	-2.12868200
H	-5.80115000	-5.27449700	-2.19594400
H	-5.95137400	-4.24353300	-0.76762600

Sum of electronic and zero-point Energies= -3149.808190

Sum of electronic and thermal Energies= -3149.750712

Sum of electronic and thermal Enthalpies -3149.749768

Sum of electronic and thermal Free Energies= -3149.906077

Basket [**3**–CH_4]

C	0.18244700	-1.36179800	4.37098200
C	-0.75076200	-0.37086500	4.50730000
C	-0.35235500	0.99292700	4.43269800
C	0.96362500	1.31375500	4.24050600
C	1.93093800	0.28157400	4.08373300
C	1.55184500	-1.03077600	4.16826100
C	-2.27171500	-0.36775800	4.65861600
H	-2.72597200	-1.28427100	5.03630900
C	-1.63526400	1.81460700	4.50488900
H	-1.52579300	2.87472500	4.73551300
C	-2.44325700	0.93092500	5.49617100
H	-1.97399500	0.86481900	6.48143300
H	-3.48823900	1.24005600	5.58710000
C	-2.79365000	0.13780300	3.31932300
C	-2.38009400	1.48402700	3.21192600
C	0.09344800	-2.88175200	4.27187400
H	-0.81244500	-3.34550300	4.66333700
C	2.29127900	-2.35538500	3.98303100
H	3.37247900	-2.33438300	4.12250800
C	1.45013900	-3.25555000	4.93079000
H	1.69330000	-4.31695400	4.83043000
H	1.51066900	-2.94371600	5.97693600
C	1.79642100	-2.88264700	2.64174800
C	0.42824500	-3.18896100	2.81281000
C	1.70405100	2.63459300	4.03743900
H	1.21745700	3.53143300	4.42208100
C	3.24226800	0.98107700	3.73757900
H	4.15416300	0.39154400	3.83759200
C	3.09017500	2.24755900	4.62508500
H	3.04765200	2.01165800	5.69174600
H	3.85758600	3.00107300	4.42798000
C	2.06088500	2.64710900	2.55695400
C	2.99696100	1.60741200	2.36315700
C	1.63075700	-3.43748200	0.36553900
C	0.28004500	-3.71212100	0.52536600
C	-3.74108100	0.26383300	1.17337000
C	-3.30424400	1.57511300	1.05160000
C	-2.61348700	2.23044800	2.06794400
C	-3.49238700	-0.50206100	2.30820400
C	1.58868600	3.42086800	1.50921400
C	3.46766700	1.27587500	1.10215200
C	-0.36590100	-3.59974400	1.75386600
C	2.43266600	-3.00518200	1.41716200
H	-2.28917100	3.26082100	1.95395000
H	-3.83109500	-1.53164600	2.37844500
H	0.87695300	4.23045100	1.64181500
H	4.17362600	0.46995700	0.92364100

H	3.48451400	-2.77963700	1.26779000
H	-1.42440500	-3.82161600	1.85557500
C	-3.71438300	2.07738600	-0.29420000
C	-4.46915700	-0.10755300	-0.07673800
N	-4.36282500	1.00387500	-0.92021200
O	-3.54615600	3.16793800	-0.78143500
O	-5.05249700	-1.13104800	-0.33542300
C	-0.27131200	-4.11700000	-0.80208600
C	1.99487400	-3.68260000	-1.06201400
N	0.80047700	-4.03491100	-1.70140200
O	-1.39451500	-4.45248800	-1.08763300
O	3.07908500	-3.61617800	-1.58703700
C	0.68587100	-4.44026900	-3.08928300
H	-0.23941200	-5.03283900	-3.12709500
C	1.80633200	-5.40149900	-3.47183900
O	2.31901000	-5.45194000	-4.55852000
O	2.09743000	-6.25882700	-2.47832100
H	2.81118200	-6.83064500	-2.80971800
C	-4.99207800	1.12480500	-2.22133100
H	-5.05818800	2.20905300	-2.39264700
C	-6.43380400	0.62860400	-2.18174500
O	-6.99437700	0.08572200	-3.09727300
O	-7.04693000	0.95384100	-1.03025200
H	-7.95430800	0.60805300	-1.09626600
C	2.97905300	2.05148100	0.05348100
C	2.08496900	3.09400500	0.25137800
C	3.27308600	1.96530700	-1.40853700
C	1.79605800	3.72555000	-1.07092400
O	4.01110700	1.20980200	-1.99117100
O	1.11646800	4.69228700	-1.31410400
N	2.50263600	2.96894600	-2.01280500
C	2.57879400	3.26170800	-3.43117600
H	3.50011700	2.76194100	-3.76384600
C	2.80969100	4.74920800	-3.67473100
O	2.37826100	5.35925900	-4.61733100
O	3.63555300	5.28880500	-2.76217100
H	3.73378700	6.22672600	-3.00252300
C	0.04549300	-0.05624200	0.84102100
H	-0.90593100	-0.49436500	1.15358300
H	0.86268100	-0.54536600	1.37697800
H	0.17991200	-0.20033000	-0.23493700
H	0.04859300	1.01273400	1.07126300
C	1.40914400	2.70307700	-4.25526800
H	1.63898000	2.97629700	-5.29208600
C	0.54980400	-3.27159300	-4.07640900
H	0.45282200	-3.74276500	-5.06163900
C	-4.18260000	0.50622800	-3.37177800
H	-4.76843300	0.71699100	-4.27468100
C	1.37309800	1.17991100	-4.13795500
H	2.34195300	0.72590100	-4.36938500
H	1.09730600	0.87304900	-3.12129200
H	0.62309600	0.76541400	-4.81927800
C	0.05682800	3.31183400	-3.88831000
H	-0.70295700	2.95341000	-4.59027400
H	-0.25478300	3.01145000	-2.88177500
H	0.07865100	4.40274500	-3.92817700
C	-0.72187000	-2.47869400	-3.77313100
H	-1.60824300	-3.12013500	-3.73206000
H	-0.63811800	-1.96518800	-2.80710900
H	-0.88250200	-1.71212100	-4.53836300
C	1.77286300	-2.35641700	-4.10020000
H	1.65916200	-1.61983800	-4.90153200
H	1.87585900	-1.80772100	-3.15714500
H	2.69483100	-2.91557200	-4.27119800

C	-4.01274600	-1.00712100	-3.25085300
H	-4.97305600	-1.51273000	-3.13270800
H	-3.52522000	-1.39202000	-4.15285100
H	-3.38031200	-1.26717300	-2.39429900
C	-2.82567000	1.20133000	-3.48184900
H	-2.92562500	2.29068100	-3.53978100
H	-2.19933300	0.96897800	-2.61127500
H	-2.29078700	0.85365100	-4.37230700

Sum of electronic and zero-point Energies= -3190.268147

Sum of electronic and thermal Energies= -3190.209231

Sum of electronic and thermal Enthalpies= -3190.208287

Sum of electronic and thermal Free Energies= -3190.361917

Basket [**3**–C_2H_6]

C	-4.43258700	-1.05022100	0.99323000
C	-4.44064900	-1.42943700	-0.32167500
C	-4.43822600	-0.44016300	-1.34457800
C	-4.48451600	0.88763000	-1.01574400
C	-4.47403200	1.27867700	0.35230600
C	-4.47542000	0.32934200	1.33805600
C	-4.32044900	-2.78184700	-1.02605500
H	-4.62795600	-3.65849100	-0.45531300
C	-4.24181200	-1.19304700	-2.65679900
H	-4.46265800	-0.64672100	-3.57411000
C	-5.08125200	-2.46287100	-2.34234400
H	-6.13852300	-2.23789800	-2.17886900
H	-4.96611200	-3.24643600	-3.09600200
C	-2.89850200	-2.79649200	-1.56379400
C	-2.83311800	-1.78782200	-2.55075300
C	-4.24219000	-1.80535000	2.30477000
H	-4.43840300	-2.87765800	2.28708300
C	-4.37922500	0.39854500	2.86313800
H	-4.71514800	1.32382000	3.33202800
C	-5.11582300	-0.91798800	3.23362400
H	-5.01117700	-1.17524600	4.29117000
H	-6.16910600	-0.91278600	2.94094600
C	-2.95016400	-0.02780400	3.16405300
C	-2.84945400	-1.38497700	2.78573700
C	-4.41664600	2.17695700	-1.83622000
H	-4.73952200	2.11079200	-2.87556700
C	-4.32417600	2.79659200	0.35384200
H	-4.54675500	3.31119500	1.28906600
C	-5.19359900	3.13243700	-0.88928700
H	-6.24080500	2.84522400	-0.75958200
H	-5.11721700	4.18018900	-1.19335900
C	-3.00638000	2.69380300	-1.60127700
C	-2.93115400	3.04431800	-0.23502200
C	-0.65706400	0.00613100	3.66379200
C	-0.54212400	-1.31369500	3.25088100
C	-0.60249500	-3.20644200	-1.82658700
C	-0.52174300	-2.18381100	-2.76098200
C	-1.63487800	-1.44473800	-3.15910500
C	-1.79188000	-3.53964700	-1.18782000
C	-1.91303400	2.76663000	-2.44846300
C	-1.73318300	3.42732900	0.34964500
C	-1.63431500	-2.05386400	2.80145600
C	-1.86312100	0.69685700	3.62433300
H	-1.54754300	-0.65586800	-3.90071600
H	-1.83153500	-4.33048600	-0.44438100
H	-1.96056800	2.51381200	-3.50363800
H	-1.63665700	3.67397100	1.40309100
H	-1.92879100	1.73571600	3.93436700
H	-1.52146100	-3.08808700	2.48896900

C	0.90056600	-2.08269700	-3.21085700
C	0.74762500	-3.82610300	-1.68614000
N	1.59804200	-3.07191100	-2.50227000
O	1.39001000	-1.32642600	-4.01309600
O	1.06891000	-4.79326200	-1.04044200
C	0.88764900	-1.72206900	3.40814000
C	0.67805100	0.47006300	4.14256100
N	1.55542400	-0.59639000	3.91317300
O	1.40355600	-2.78595000	3.16900500
O	0.97114300	1.52231800	4.65385500
C	2.93011900	-0.64544500	4.37812800
H	3.15726100	-1.71888400	4.44987500
C	3.04163600	-0.10678000	5.80184200
O	3.98005800	0.51394800	6.22570000
O	2.00383200	-0.48854100	6.56713100
H	2.16327100	-0.11173500	7.44997800
C	2.98125500	-3.41006500	-2.78349600
H	3.19155700	-2.92624500	-3.74819300
C	3.13144400	-4.90807700	-3.03243000
O	4.09295300	-5.55925800	-2.71997300
O	2.09781700	-5.40829700	-3.73222100
H	2.27921700	-6.35722400	-3.84738000
C	-0.63345600	3.48201900	-0.50552200
C	-0.72506700	3.18230400	-1.85717900
C	0.78574200	3.84880700	-0.21102400
C	0.61479600	3.39315600	-2.48072300
O	1.28269600	4.17125600	0.83998400
O	0.92609700	3.31540000	-3.64337500
N	1.47057500	3.74302400	-1.43024900
C	2.84654800	4.17430300	-1.59655500
H	3.05710800	4.77145600	-0.69774100
C	2.97575700	5.13962200	-2.77062600
O	3.92946800	5.20249900	-3.50038900
O	1.93500700	5.98787700	-2.84212800
H	2.10564100	6.56529400	-3.60644900
C	-1.06116300	0.00667700	-0.00471600
H	-1.36906300	-1.02808200	-0.18473200
H	-1.53554900	0.33664500	0.92457300
H	-1.46596600	0.61808600	-0.81719200
C	3.86903700	3.03173000	-1.66134300
H	4.83869200	3.52922200	-1.78320800
C	3.94799900	-0.00032100	3.42864800
H	4.91554500	-0.11722900	3.93127400
C	3.98809500	-2.88372300	-1.75188600
H	4.96523300	-3.22613700	-2.11306200
C	3.86836600	2.25995000	-0.34314900
H	3.97643700	2.92541500	0.51894800
H	2.93179200	1.70166400	-0.21977800
H	4.68806000	1.53422900	-0.32700300
C	3.65976700	2.09369500	-2.84880400
H	4.49732000	1.39148700	-2.90493600
H	2.74156000	1.50473900	-2.73605100
H	3.60200000	2.63975800	-3.79260300
C	3.97944100	-0.76270600	2.10551000
H	4.12219800	-1.83720200	2.25724900
H	3.04073400	-0.62406200	1.55456000
H	4.79060900	-0.39021100	1.47137500
C	3.70220300	1.48986900	3.19936900
H	4.53123100	1.90742700	2.61924900
H	2.78148800	1.65668600	2.62788000
H	3.62515200	2.03836500	4.14042400
C	3.77048000	-3.44792900	-0.34896500
H	3.72510200	-4.53876500	-0.35319200
H	4.59776500	-3.13761800	0.29678100

H	2.84288500	-3.06668600	0.09388200
C	3.96799000	-1.35649500	-1.74173400
H	4.10356700	-0.94059000	-2.74478700
H	3.01337400	-0.98205500	-1.35101900
H	4.76143000	-0.96978400	-1.09379100
C	0.45786500	0.12769600	0.07837000
H	0.92106000	0.05127600	-0.91377000
H	0.75939400	1.08955400	0.51261400
H	0.88596500	-0.66447400	0.70539800

Sum of electronic and zero-point Energies= -3229.532621

Sum of electronic and thermal Energies= -3229.472374

Sum of electronic and thermal Enthalpies= -3229.471430

Sum of electronic and thermal Free Energies= -3229.625047

Basket [**3**–C_3H_8]

C	-4.58101500	0.68786300	0.22879700
C	-4.47237500	-0.10637900	1.33838800
C	-4.26795400	-1.50763300	1.19403000
C	-4.17896200	-2.06150700	-0.05458800
C	-4.28111500	-1.23472400	-1.20801300
C	-4.47285600	0.11321300	-1.06879900
C	-4.39927400	0.18435800	2.83598600
H	-4.81245400	1.13604700	3.17188900
C	-4.07085900	-2.05839100	2.60559600
H	-4.18761500	-3.13527500	2.73227000
C	-5.03651600	-1.12242300	3.38402200
H	-6.07987600	-1.24407800	3.08043000
H	-4.93712000	-1.21950900	4.46877100
C	-2.93942500	-0.07903300	3.19703800
C	-2.73647100	-1.46925100	3.05567200
C	-4.73714200	2.19334900	0.01961600
H	-5.13235800	2.76373800	0.86098800
C	-4.54311700	1.27392700	-2.05667600
H	-4.75968100	1.01928600	-3.09478000
C	-5.55850900	2.17888000	-1.30160900
H	-5.65809200	3.17166300	-1.74928000
H	-6.53861000	1.70818700	-1.18588800
C	-3.26971600	2.08419500	-1.81876600
C	-3.39731400	2.66367200	-0.53674800
C	-3.87838400	-3.47009400	-0.56322500
H	-4.05060200	-4.28877100	0.13629500
C	-4.04439400	-2.14578100	-2.41021100
H	-4.36668700	-1.76730100	-3.38085000
C	-4.71086100	-3.44586900	-1.87634600
H	-5.78286200	-3.32818000	-1.69599800
H	-4.51982000	-4.31286800	-2.51497500
C	-2.47724000	-3.38524300	-1.16286200
C	-2.57946100	-2.56090800	-2.30473700
C	-1.15161900	3.08294200	-2.03976700
C	-1.28724900	3.66831600	-0.78845300
C	-0.65966200	0.19029900	3.70628100
C	-0.45967000	-1.17691100	3.56244400
C	-1.48985000	-2.05114100	3.22966200
C	-1.90526000	0.78460500	3.52353800
C	-1.26649600	-3.91985200	-0.74894600
C	-1.47168100	-2.22116300	-3.06638700
C	-2.41087500	3.47014700	0.00888300
C	-2.13657300	2.27044400	-2.59539600
H	-1.30865200	-3.11578700	3.11264200
H	-2.03882200	1.85745400	3.62986200
H	-1.16795600	-4.56183500	0.12174800
H	-1.52463700	-1.57957400	-3.94144700
H	-2.01196200	1.83053400	-3.58091300

H	-2.49791500	3.93499700	0.98680700
C	0.98684800	-1.46706800	3.80360100
C	0.65069200	0.81528900	4.06147100
N	1.58330200	-0.22322900	4.04486800
O	1.56020300	-2.52769300	3.79842900
O	0.90809600	1.96609500	4.32254100
C	-0.08128300	4.51329200	-0.53676100
C	0.15536100	3.51702500	-2.62055000
N	0.74994500	4.33712300	-1.65234600
O	0.16080600	5.22772500	0.40466800
O	0.62719000	3.25356000	-3.69931700
C	1.95529300	5.12322000	-1.85246600
H	1.85278500	5.96314000	-1.15002700
C	1.96944200	5.75225200	-3.24256800
O	2.95770800	5.91857100	-3.90735500
O	0.75275400	6.19490000	-3.60632200
H	0.85584300	6.58126300	-4.49355800
C	2.96237100	-0.05914500	4.45189400
H	3.37220100	-1.07984300	4.44920400
C	3.02414000	0.43948700	5.89563000
O	3.90439300	1.12075200	6.35216800
O	1.98860800	-0.00640300	6.62955000
H	2.11774900	0.34847800	7.52670000
C	-0.26202800	-2.76520100	-2.64493600
C	-0.16419200	-3.59307500	-1.53398700
C	1.10143500	-2.61331200	-3.23851100
C	1.26310700	-4.01643900	-1.39653700
O	1.43850200	-1.98616100	-4.21243200
O	1.76614100	-4.77268100	-0.60110700
N	1.95305500	-3.36483400	-2.42141600
C	3.35060800	-3.60438700	-2.71884100
H	3.50832000	-3.13320700	-3.70009500
C	3.58203200	-5.10514300	-2.90099100
O	4.58181900	-5.69706500	-2.59096500
O	2.53662200	-5.70177100	-3.50289700
H	2.77025700	-6.64320700	-3.58257100
C	0.45326300	-0.33303900	0.08315800
H	0.73724400	-1.32193300	-0.29901300
H	0.77428700	-0.30740700	1.13251100
C	-1.06040200	-0.17044700	0.00332200
H	-1.58455500	-0.97671600	0.52793900
H	-1.37450800	0.78330700	0.44691400
H	-1.39563000	-0.17433100	-1.04076000
C	1.18697000	0.74967000	-0.70117100
H	0.89906700	1.74525500	-0.33892500
H	2.27463500	0.66394200	-0.60410300
H	0.93696300	0.70056300	-1.77011800
C	4.33236300	-2.98978200	-1.70215800
H	4.39117600	-3.66965100	-0.84459800
C	3.26103700	4.38445200	-1.52734300
H	4.05702000	5.10836500	-1.74032800
C	3.80929900	0.82944600	3.51421500
H	3.67051100	1.86932300	3.82883800
C	3.82956700	-1.62475400	-1.23350400
H	3.60082900	-0.97517600	-2.08875300
H	2.92569300	-1.71240600	-0.62302200
H	4.59511200	-1.12860900	-0.62772100
C	5.71959600	-2.85938400	-2.33601000
H	6.43278100	-2.47242800	-1.60202800
H	6.08897500	-3.82096100	-2.69683900
H	5.68836000	-2.15265300	-3.17480300
C	3.30049700	4.02355000	-0.04239100
H	3.13222400	4.89639600	0.59664600
H	2.53123900	3.28072600	0.19905500

H	4.27159700	3.58843200	0.21469700
C	3.48238400	3.15331800	-2.40448400
H	4.44995800	2.69916900	-2.16575400
H	2.70759300	2.40052000	-2.22602100
H	3.47089800	3.40984100	-3.46615300
C	3.35171100	0.68632300	2.06370700
H	2.36985400	1.14299300	1.90497400
H	4.06111400	1.18576100	1.39507600
H	3.29128500	-0.36931700	1.76586600
C	5.28662900	0.45809300	3.65807500
H	5.61399500	0.52335000	4.69791500
H	5.45853800	-0.56289900	3.29469000
H	5.90636400	1.13424100	3.06143600

Sum of electronic and zero-point Energies= -3268.795185

Sum of electronic and thermal Energies= -3268.732610

Sum of electronic and thermal Enthalpies= -3268.731666

Sum of electronic and thermal Free Energies= -3268.894205

[1] Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.