# Assessment of Dispersion-Improved Exchange-Correlation Functionals for the Simulation of $CO_2$ Binding by Alcoholamines

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Supplementary Material

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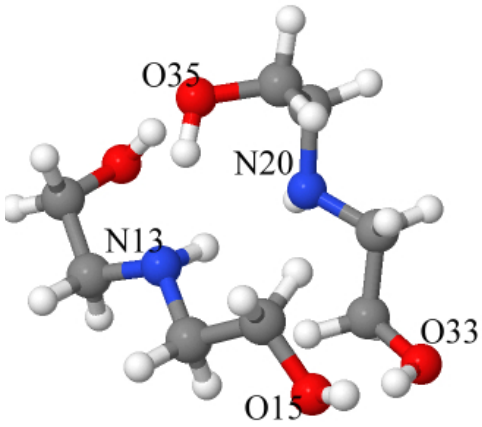


Figure S1. Local minimum structure of DEA dimer at M06-2X levels.

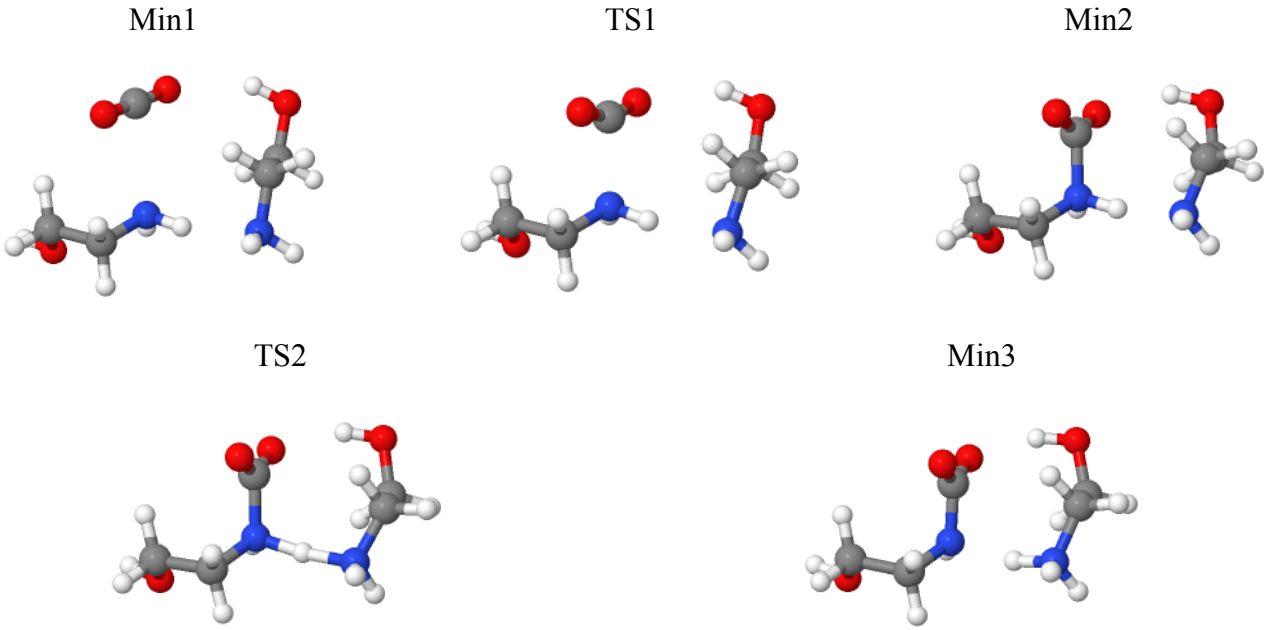


Figure S2. Schematic presentation of trimolecular reaction pathway.

Table S1. Binding energy (in kcal/mol) of complexes *a-l* using MP2/ATZ optimized geometries.

| | *a* | *b* | *c* | *d* | *e* | *f* |
|---|---|---|---|---|---|---|
| ωB97 | -5.69 | -7.34 | -8.60 | -5.38 | -8.61 | -5.26 |
| ωB97X | -5.63 | -7.32 | -8.44 | -5.21 | -8.49 | -5.07 |
| ωB97XD | -4.98 | -6.85 | -8.10 | -5.08 | -8.74 | -5.29 |
| LC-ωPBE | -4.39 | -6.08 | -6.69 | -3.37 | -6.71 | -3.01 |
| CAM-B3LYP | -5.23 | -6.79 | -7.54 | -3.93 | -7.34 | -3.50 |
| B3LYP-GD2 | -5.32 | -7.13 | -8.92 | -5.41 | -9.28 | -5.59 |
| B3LYP-GD3 | -5.25 | -7.01 | -8.51 | -5.01 | -8.95 | -5.16 |
| BLYP-D | -4.93 | -6.81 | -8.54 | -5.12 | -8.93 | -5.27 |
| B97-D | -4.31 | -6.32 | -7.81 | -4.73 | -8.47 | -4.96 |
| M06-2X | -5.12 | -6.59 | -7.99 | -4.60 | -8.12 | -4.81 |
| M05-2X | -5.19 | -6.63 | -7.91 | -4.50 | -8.05 | -4.58 |
| M06HF | -4.76 | -6.45 | -8.06 | -4.10 | -8.41 | -4.62 |
| M06-L | -4.58 | -6.23 | -7.37 | -4.31 | -7.44 | -4.44 |
| B2PLYP | -4.34 | -5.64 | -5.87 | -2.76 | -5.57 | -2.14 |
| B2PLYPD | -4.76 | -6.17 | -7.17 | -3.97 | -7.19 | -3.78 |
| | *g* | *h* | *i* | *j* | *k* | *l* |
| ωB97 | -4.81 | -5.63 | -11.96 | -3.76 | -4.85 | -4.51 |
| ωB97X | -4.56 | -5.28 | -10.92 | -3.57 | -4.45 | -3.97 |
| ωB97XD | -4.88 | -6.32 | -13.93 | -2.86 | -3.89 | -3.88 |
| LC-ωPBE | -2.23 | -2.45 | -5.88 | -2.11 | -2.33 | -1.33 |
| CAM-B3LYP | -2.81 | -2.93 | -6.67 | -2.64 | -3.02 | -1.94 |
| B3LYP-GD2 | -5.24 | -6.57 | -14.99 | -3.16 | -4.50 | -4.70 |
| B3LYP-GD3 | -4.69 | -5.94 | -13.45 | -3.17 | -4.47 | -4.61 |
| BLYP-D | -5.01 | -6.27 | -14.47 | -2.73 | -3.97 | -4.21 |
| B97-D | -4.64 | -6.00 | -13.46 | -2.39 | -3.36 | -3.63 |
| M06-2X | -4.20 | -5.27 | -12.04 | -3.47 | -4.74 | -4.86 |
| M05-2X | -3.88 | -4.80 | -10.47 | -3.35 | -4.44 | -4.33 |
| M06HF | -3.62 | -4.80 | -10.90 | -3.35 | -4.58 | -4.73 |
| M06-L | -4.09 | -5.21 | -12.33 | -2.48 | -3.53 | -3.89 |
| B2PLYP | -1.43 | -1.20 | -2.50 | -2.05 | -1.97 | -0.47 |
| B2PLYPD | -3.23 | -3.84 | -8.41 | -2.70 | -3.36 | -2.70 |

Table S2. Binding energy (in kcal/mol) of complexes *a-l* using the corresponding DFT optimized geometries.

| | *a* | *b* | *c* | *d* | *e* | *f* |
|---|---|---|---|---|---|---|
| ωB97 | -5.71 | -7.34 | -8.58 | -5.37 | -8.55 | -5.29 |
| ωB97X | -5.64 | -7.30 | -8.37 | -5.15 | -8.38 | -5.09 |
| ωB97XD | -4.98 | -6.84 | -8.06 | -5.09 | -8.62 | -5.36 |
| LC-ωPBE | -4.40 | -6.09 | -6.67 | -3.35 | -6.65 | -3.20 |
| CAM-B3LYP | -5.27 | -6.83 | -7.54 | -3.89 | -7.36 | -3.70 |
| B3LYP-GD2 | -5.41 | -7.25 | -9.05 | -5.43[1] | -9.46 | -5.68 |
| B3LYP-GD3 | -5.29 | -7.08 | -8.58 | -5.05 | -9.00 | -5.29 |
| BLYP-D | -5.14 | -7.12 | -8.99 | -3.72 | -9.46 | -5.58 |
| B97-D | -4.46 | -6.49 | -8.07 | -4.63 | -8.73 | -5.12 |
| M06-2X | -5.13 | -6.58 | -7.98 | -4.57 | -8.09 | -4.90 |
| M05-2X | -5.19 | -6.61 | -7.86 | -4.53 | -7.97 | -4.58 |
| M06HF | -4.78 | -6.47 | -8.26 | -4.26 | -8.78 | -4.76 |
| M06-L | -4.58 | -6.20 | -7.34 | -4.34 | -7.35 | -4.60 |
| B2PLYP | -4.35 | -5.66 | -6.00 | -2.87 | -5.72 | -2.61 |
| B2PLYPD | -4.75 | -6.18 | -7.18 | NA | -7.18 | -3.83 |

| | *g* | *h* | *i* | *j* | *k* | *l* |
|---|---|---|---|---|---|---|
| ωB97 | -4.87 | -5.71 | -12.28 | -3.84 | -4.33 | -4.51 |
| ωB97X | -4.55 | -5.29 | -11.30 | -3.61 | -4.47 | -4.00 |
| ωB97XD | -4.86 | -6.46 | -14.13 | -2.89 | -3.51 | -4.06 |
| LC-ωPBE | -2.59 | -3.04 | -6.80 | -2.12 | -2.48 | -1.64 |
| CAM-B3LYP | -3.09 | -3.49 | -7.86 | -2.66 | -3.12 | -2.18 |
| B3LYP-GD2 | -5.36 | -6.79 | -15.62 | -3.20 | -4.56 | -4.82 |
| B3LYP-GD3 | -4.74 | -6.08 | -13.99 | -3.21 | -4.55 | -4.71 |
| BLYP-D | -5.19 | -6.51 | -15.75 | -2.79 | -4.11 | -4.44 |
| B97-D | -4.77 | -6.11 | -14.36 | -2.47 | -3.53 | -3.91 |
| M06-2X | -4.26 | -11.03 | -21.12 | -3.57 | -4.22 | -4.89 |
| M05-2X | -3.90 | -4.83 | -10.54 | -3.40 | -4.57 | -4.40 |
| M06HF | -3.62 | -4.85 | -11.04 | -3.60 | -4.39 | -5.25 |
| M06-L | -4.11 | -5.27 | -12.71 | -2.48 | -3.57 | -3.89 |
| B2PLYP | -2.10 | -2.33 | -4.43 | -2.09 | -2.33 | -1.11 |
| B2PLYPD | -3.21 | -3.80 | -8.49 | -2.72 | -3.37 | -2.77 |

[1] Used NWChem optimized geometries.

Optimized Cartesian coordinate (in Å) of all complexes of C1 Database at MP2/ATZ

a. $(H_2O)_2$

| | | | |
|---|---|---|---|
| O | -1.51139800 | -0.00295600 | -0.12206000 |
| H | -0.55881500 | -0.00033800 | 0.05332900 |
| H | -1.91607100 | 0.01852700 | 0.74870900 |
| O | 1.38638600 | 0.00220900 | 0.11201500 |
| H | 1.73992800 | -0.76695200 | -0.34564000 |
| H | 1.73505900 | 0.75473500 | -0.37603700 |

b. $NH_3(H_2O)$

| | | | |
|---|---|---|---|
| N | -1.37577400 | 0.02221200 | 0.00002300 |
| H | -1.70581100 | -0.28116100 | 0.90799100 |
| H | -1.63464800 | -0.69850600 | -0.66274500 |
| H | -1.90371100 | 0.85058500 | -0.24481300 |
| O | 1.54474400 | -0.10600700 | -0.00011400 |
| H | 0.58228200 | 0.04997800 | -0.00033800 |
| H | 1.93435300 | 0.77167200 | 0.00066200 |

c. $MEA(H_2O)$

| | | | |
|---|---|---|---|
| N | 0.83508500 | 1.32273500 | 0.18645200 |
| H | 1.18009000 | 2.12662500 | -0.32449000 |
| H | 0.72788100 | 1.62301300 | 1.14928000 |
| C | -0.46579500 | 0.90246900 | -0.35453900 |
| C | -0.91052100 | -0.36744500 | 0.33976100 |
| H | -0.34532900 | 0.70029200 | -1.41787900 |
| H | -1.24962100 | 1.65641200 | -0.24171700 |
| H | -0.20924000 | -1.17350100 | 0.12069900 |
| H | -0.92368900 | -0.20584600 | 1.42383100 |
| O | -2.22034700 | -0.66032900 | -0.14107300 |
| H | -2.44646500 | -1.55389900 | 0.13333900 |
| O | 2.28339300 | -1.13700500 | -0.09552400 |
| H | 1.93981100 | -0.22721200 | 0.01909200 |
| H | 3.23449300 | -1.03650100 | -0.18587600 |

d. $MEA(NH_3)$

| | | | |
|---|---|---|---|
| N | -0.06462000 | 1.30115300 | -0.55658200 |
| H | -0.06364900 | 2.30868900 | -0.66114600 |
| H | 0.33024300 | 0.91933600 | -1.40964600 |
| H | -1.95022100 | 0.17897600 | -0.20349700 |
| H | -3.08829500 | -0.86199500 | -0.74579300 |
| N | -2.61016900 | -0.54151900 | 0.08742700 |

| | | | |
|---|---|---|---|
| H | -3.31193600 | -0.09285400 | 0.66338600 |
| C | 0.79888700 | 0.90360300 | 0.55942300 |
| C | 0.87644700 | -0.60325600 | 0.61638900 |
| H | 0.36210000 | 1.26585300 | 1.49107300 |
| H | 1.81599100 | 1.30354900 | 0.48364900 |
| H | 1.48142900 | -0.90916000 | 1.47405700 |
| H | -0.12816500 | -1.01836600 | 0.70928400 |
| O | 1.49018200 | -1.03084600 | -0.60612500 |
| H | 1.30256500 | -1.96678100 | -0.72314900 |

e. DEA($H_2O$)

| | | | |
|---|---|---|---|
| C | -2.43300000 | -0.06993600 | 0.35237300 |
| C | -1.21506200 | -0.73233600 | -0.25510400 |
| H | -2.41183100 | -0.18920000 | 1.44147800 |
| H | -2.42069500 | 0.99794300 | 0.12500200 |
| H | -1.27452000 | -1.81617600 | -0.09849100 |
| H | -1.21163300 | -0.55629400 | -1.33180100 |
| C | 1.21487800 | -0.73241600 | -0.25512200 |
| C | 2.43287300 | -0.07012100 | 0.35236200 |
| H | 1.27425300 | -1.81626400 | -0.09852500 |
| H | 1.21145600 | -0.55635400 | -1.33181500 |
| H | 2.42068200 | 0.99774900 | 0.12495500 |
| H | 2.41166200 | -0.18934900 | 1.44147100 |
| N | -0.00007100 | -0.14668200 | 0.30873000 |
| H | -0.00006900 | -0.30522100 | 1.31280400 |
| O | -3.57405200 | -0.71497300 | -0.20490700 |
| H | -4.36023400 | -0.24921900 | 0.09584800 |
| O | 3.57387800 | -0.71530100 | -0.20485600 |
| H | 4.36008700 | -0.24945000 | 0.09568000 |
| O | 0.00056500 | 2.68498300 | -0.09757800 |
| H | -0.00014400 | 2.84186100 | -1.04563700 |
| H | 0.00022100 | 1.70792900 | -0.00040500 |

f. DEA($NH_3$)

| | | | |
|---|---|---|---|
| N | -0.09342300 | -0.04690700 | 0.15165500 |
| H | -0.19134800 | -0.81765300 | -0.50319700 |
| H | 0.50706400 | 1.91709700 | -0.44816300 |
| N | 1.02607400 | 2.79438800 | -0.51126700 |
| H | 0.94426600 | 3.12335800 | -1.46558000 |
| C | -1.31398800 | 0.04511100 | 0.93798700 |
| C | -2.50835000 | 0.19560900 | 0.02829300 |

| | | | |
|---|---|---|---|
| H | -1.24953000 | 0.92232100 | 1.58758600 |
| H | -1.46503600 | -0.83368300 | 1.58155300 |
| H | -3.41429400 | 0.33601200 | 0.62430400 |
| H | -2.36519300 | 1.06566300 | -0.61762700 |
| O | -2.59248400 | -1.00114900 | -0.74729200 |
| H | -3.25442900 | -0.87490900 | -1.43374200 |
| C | 1.07722500 | -0.30075500 | 0.98151800 |
| C | 2.29246600 | -0.51282300 | 0.11296800 |
| H | 0.94169100 | -1.17682600 | 1.63193000 |
| H | 1.25115600 | 0.56889100 | 1.62007800 |
| H | 3.17501100 | -0.65209300 | 0.74303900 |
| H | 2.44017800 | 0.36297300 | -0.52134900 |
| O | 2.04280700 | -1.68329700 | -0.67218100 |
| H | 2.71537700 | -1.73633400 | -1.35766300 |
| H | 0.54982900 | 3.47553200 | 0.06731600 |

g. $(MEA)_2$

| | | | |
|---|---|---|---|
| N | -1.77075600 | 1.72820200 | 0.27185800 |
| H | -2.04681700 | 2.62051800 | -0.11996300 |
| H | -1.89971500 | 1.80908300 | 1.27441900 |
| C | -2.62465100 | 0.65833200 | -0.25752600 |
| C | -2.09411500 | -0.67982100 | 0.21130800 |
| H | -2.58214700 | 0.69051800 | -1.34570600 |
| H | -3.67517500 | 0.74022400 | 0.03779000 |
| H | -1.10259500 | -0.84576400 | -0.21338400 |
| H | -2.01266500 | -0.67554400 | 1.30508300 |
| O | -3.02581400 | -1.67181400 | -0.21709000 |
| H | -2.60777300 | -2.53312600 | -0.12759200 |
| N | 1.03729200 | 0.48201200 | -0.63639200 |
| H | 0.24558600 | 1.09279200 | -0.44622600 |
| H | 1.69597600 | 0.99421700 | -1.21186000 |
| C | 1.69266200 | 0.12701400 | 0.61769700 |
| C | 2.89458600 | -0.74184400 | 0.34000200 |
| H | 0.99080700 | -0.44068600 | 1.23293000 |
| H | 2.02426000 | 0.99094700 | 1.20715800 |
| H | 3.33361500 | -1.08980200 | 1.27941100 |
| H | 2.58530200 | -1.60320400 | -0.25726900 |
| O | 3.83213100 | 0.06057700 | -0.38384400 |
| H | 4.52415900 | -0.51385500 | -0.72446700 |

h. MEA(DEA)

| | | | |
|---|---|---|---|
| N | -1.34367400 | 0.06624700 | 0.11023100 |

| | | | |
|---|---|---|---|
| H | -2.14721500 | 0.15532000 | -0.50486000 |
| H | 0.59212100 | -0.38729500 | -0.61299700 |
| N | 1.56550900 | -0.69090700 | -0.57283600 |
| H | 1.99618600 | -0.46331200 | -1.46217800 |
| C | -1.24520000 | 1.26797900 | 0.92447800 |
| C | -1.10256400 | 2.48191800 | 0.04003700 |
| H | -0.35926300 | 1.18848900 | 1.55993200 |
| H | -2.11567300 | 1.40328000 | 1.58269800 |
| H | -0.95566700 | 3.37495600 | 0.65387900 |
| H | -0.23764200 | 2.35082800 | -0.61569600 |
| O | -2.30603900 | 2.58372500 | -0.72290800 |
| H | -2.17931200 | 3.24921700 | -1.40586000 |
| C | 2.26341200 | 0.04140100 | 0.47776400 |
| C | 3.72841800 | -0.32039300 | 0.47330800 |
| H | 1.84353900 | -0.24248900 | 1.44575100 |
| H | 2.18369300 | 1.13370100 | 0.38975100 |
| H | 4.23636900 | 0.14977500 | 1.32012000 |
| H | 3.82944900 | -1.40594300 | 0.54623800 |
| O | 4.27197900 | 0.15371600 | -0.76250600 |
| H | 5.15051400 | -0.22214600 | -0.87145000 |
| C | -1.50765700 | -1.13623900 | 0.91465800 |
| C | -1.69304700 | -2.33564100 | 0.01825100 |
| H | -2.36072500 | -1.06522100 | 1.60483800 |
| H | -0.60399000 | -1.28303500 | 1.51230000 |
| H | -1.75586400 | -3.24360100 | 0.62418900 |
| H | -0.83948000 | -2.41476700 | -0.65814100 |
| O | -2.90813600 | -2.12775600 | -0.70771700 |
| H | -2.95249000 | -2.77675800 | -1.41621400 |

i. $(DEA)_2$

| | | | |
|---|---|---|---|
| C | -0.91182400 | 2.02579800 | 0.95484100 |
| C | 0.08247000 | 2.22682600 | -0.16965800 |
| H | -1.30478600 | 1.00492500 | 0.91428100 |
| H | -0.40798400 | 2.15772000 | 1.91559700 |
| H | -0.46361400 | 2.29313900 | -1.12136600 |
| H | 0.60015500 | 3.17796800 | -0.02874400 |
| C | 2.14784000 | 1.35470700 | -1.09091100 |
| C | 3.10305600 | 0.18629800 | -1.07272300 |
| H | 1.79003200 | 1.50650600 | -2.11969800 |
| H | 2.69453600 | 2.25391900 | -0.79577200 |
| H | 3.97562400 | 0.42041900 | -1.68834800 |
| H | 3.42371200 | -0.00766800 | -0.04632600 |

| | | | |
|---|---|---|---|
| N | 1.05593200 | 1.14368500 | -0.15157100 |
| H | 0.57387600 | 0.26770400 | -0.38429300 |
| O | -1.95494200 | 2.98119300 | 0.77362500 |
| H | -2.55586100 | 2.91601100 | 1.52228900 |
| O | 2.41236500 | -0.95359500 | -1.60225500 |
| H | 3.01350100 | -1.70415100 | -1.55555200 |
| H | 0.04474300 | -1.87545500 | -1.04751000 |
| N | -0.30691600 | -1.52396000 | -0.16346000 |
| C | 0.31307000 | -2.27166700 | 0.93598800 |
| C | 0.49104100 | -1.41706100 | 2.18275300 |
| H | 1.30301600 | -2.59964200 | 0.61747500 |
| H | -0.27755200 | -3.16491100 | 1.18656600 |
| H | -0.44408400 | -0.88566000 | 2.40030500 |
| H | 0.69739800 | -2.07062900 | 3.03170700 |
| C | -1.76202100 | -1.59423000 | -0.14517900 |
| C | -2.33540800 | -0.73315300 | -1.25006300 |
| H | -2.12129200 | -1.22004000 | 0.81559900 |
| H | -2.14217300 | -2.61918800 | -0.25250600 |
| H | -2.03921700 | 0.30830700 | -1.09958200 |
| H | -1.94009000 | -1.06517500 | -2.21673000 |
| O | -3.75145300 | -0.87893100 | -1.20251200 |
| H | -4.13927800 | -0.25785600 | -1.82672000 |
| O | 1.58256900 | -0.52170700 | 2.09564400 |
| H | 1.39857200 | 0.14489000 | 1.39824000 |

j. $NH_3(CO_2)$

| | | | |
|---|---|---|---|
| N | -1.99585400 | -0.01672300 | 0.00001200 |
| H | -2.33773100 | 0.93627400 | -0.01514100 |
| H | -2.39643600 | -0.45782700 | 0.81877300 |
| C | 0.94105400 | 0.00512400 | 0.00000600 |
| O | 0.94355400 | 1.17539700 | 0.00000600 |
| O | 0.98841300 | -1.16391500 | 0.00000700 |
| H | -2.39691400 | -0.48397900 | -0.80385400 |

k. $MEA(CO_2)$

| | | | |
|---|---|---|---|
| N | 0.22347900 | 1.20788300 | -0.27534900 |
| H | -0.08640500 | 2.15689300 | -0.10263000 |
| H | 0.71878200 | 1.22303300 | -1.16050300 |
| C | 1.15396100 | 0.77602800 | 0.76852100 |
| C | 1.73476300 | -0.56463500 | 0.39219000 |
| H | 0.60669900 | 0.66527800 | 1.70548600 |
| H | 1.98073400 | 1.47525700 | 0.93513900 |

| | | | |
|---|---|---|---|
| H | 2.38162300 | -0.92752900 | 1.19502400 |
| H | 0.92495900 | -1.27918600 | 0.23184700 |
| O | 2.48422300 | -0.36793600 | -0.81090000 |
| H | 2.73629400 | -1.22936900 | -1.15653500 |
| C | -2.14257000 | -0.37130600 | -0.00589300 |
| O | -2.69509300 | 0.14005500 | -0.90065000 |
| O | -1.64327700 | -0.91895600 | 0.90177600 |

l. DEA($CO_2$)

| | | | |
|---|---|---|---|
| C | 2.42992700 | -0.48845800 | -0.43643100 |
| C | 1.20897400 | -1.06560100 | 0.24603300 |
| H | 2.41216300 | -0.74163700 | -1.50237100 |
| H | 2.42055300 | 0.60083900 | -0.34621500 |
| H | 1.28734900 | -2.16049800 | 0.25352000 |
| H | 1.18825700 | -0.73035300 | 1.28400000 |
| C | -1.20939100 | -1.06535600 | 0.24586000 |
| C | -2.43012000 | -0.48781400 | -0.43666600 |
| H | -1.28805500 | -2.16023300 | 0.25321900 |
| H | -1.18869000 | -0.73021700 | 1.28385900 |
| H | -2.42052000 | 0.60146100 | -0.34621300 |
| H | -2.41225600 | -0.74078200 | -1.50265500 |
| N | -0.00011300 | -0.58227700 | -0.41147600 |
| H | -0.00007600 | -0.90548400 | -1.37470000 |
| O | 3.57236500 | -1.05156500 | 0.20003200 |
| H | 4.35972200 | -0.65502700 | -0.18502800 |
| O | -3.57277700 | -1.05079700 | 0.19951500 |
| H | -4.35999000 | -0.65395100 | -0.18552200 |
| C | 0.00031300 | 2.15680500 | 0.23863100 |
| O | -0.00077300 | 1.80615300 | 1.35631400 |
| O | 0.00141200 | 2.56792700 | -0.85729000 |

Table S3. Summary of $\Delta E^{CCSD(T)}_{CBS(TZ\rightarrow QZ)}$ and $\Delta E^{CCSD(T)}_{CBS(DZ\rightarrow TZ)}$ calculations where the values of ΔE are in kcal/mol.

| | E[CCSD(T)] | ΔE[CCSD(T)] | E[HF] | ΔE[HF] | E2 | ΔE2 | $\Delta E^{CCSD(T)}_{CBS(TZ\rightarrow QZ)}$ | $\Delta E^{CCSD(T)}_{CBS(DZ\rightarrow TZ)}$ |
|---|---|---|---|---|---|---|---|---|
| ***a*** | $(H_2O)_2$ | | | | | | | |
| | **(aVQZ)** | | | | | | | |
| | **-152.73528** | **-4.960** | **-152.13679** | **-3.640** | **-0.59848** | **-1.320** | **-5.06** | |
| | **-76.36377** | | **-76.06563** | | **-0.29814** | | | |
| | **-76.36360** | | **-76.06537** | | **-0.29824** | | | |
| | **(aVTZ)** | | | | | | | |
| | **-152.69296** | **-4.778** | **-152.12609** | **-3.602** | **-0.56687** | **-1.176** | | -4.95 |
| | **-76.34276** | | **-76.06031** | | **-0.28246** | | | |
| | **-76.34259** | | **-76.06005** | | **-0.28254** | | | |
| | (aVDZ) | | | | | | | |
| | -152.55616 | -4.374 | -152.08813 | -3.616 | -0.46803 | -0.758 | | |
| | -76.27490 | | -76.04141 | | -0.23349 | | | |
| | -76.27429 | | -76.04096 | | -0.23333 | | | |
| ***b*** | $NH_3(H_2O)$ | | | | | | | |
| | **(aVQZ)** | | | | | | | |
| | **-132.86967** | **-6.468** | **-132.29610** | **-4.481** | **-0.57357** | **-1.987** | **-6.60** | |
| | **-76.36348** | | **-76.06499** | | **-0.29849** | | | |
| | **-56.49589** | | **-56.22397** | | **-0.27192** | | | |
| | **(aVTZ)** | | | | | | | |
| | **-132.83341** | **-6.283** | **-132.28717** | **-4.472** | **-0.54624** | **-1.811** | | -6.52 |
| | **-76.34251** | | **-76.05969** | | **-0.28282** | | | |
| | **-56.48088** | | **-56.22035** | | **-0.26053** | | | |
| | (aVDZ) | | | | | | | |
| | -132.70998 | -5.669 | -132.25366 | -4.429 | -0.45632 | -1.240 | | |
| | -76.27434 | | -76.04066 | | -0.23369 | | | |
| | -56.42660 | | -56.20594 | | -0.22066 | | | |
| ***c*** | $MEA(H_2O)$ | | | | | | | |
| | **(aVQZ)** | | | | | | | |
| | **-286.51050** | **-7.761** | **-285.27521** | **-4.297** | **-1.23530** | **-3.464** | **-7.93** | |
| | **-210.13471** | | **-209.20366** | | **-0.93104** | | | |
| | **-76.36343** | | **-76.06469** | | **-0.29873** | | | |
| | **(aVTZ)** | | | | | | | |
| | **-286.43504** | **-7.514** | **-285.25691** | **-4.283** | **-1.17813** | **-3.231** | | -7.85 |
| | **-76.34263** | | **-76.05944** | | **-0.28319** | | | |
| | **-210.08044** | | **-209.19065** | | **-0.88979** | | | |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | (aVDZ) | | | | | | | |
| | -286.17555 | -6.733 | -285.18824 | -4.300 | -0.98731 | -2.433 | | |
| | -76.27496 | | -76.04075 | | -0.23421 | | | |
| | -209.88986 | | -209.14064 | | -0.74922 | | | |
| ***d*** | MEA($NH_3$) | | | | | | | |
| | **(aVQZ)** | | | | | | | |
| | **-266.64030** | **-4.695** | **-265.43129** | **-1.709** | **-1.20901** | **-2.987** | **-4.80** | |
| | **-56.49581** | | **-56.22375** | | **-0.27206** | | | |
| | **-210.13701** | | **-209.20481** | | **-0.93219** | | | |
| | **(aVTZ)** | | | | | | | |
| | **-266.57082** | **-4.534** | **-265.41465** | **-1.691** | **-1.15617** | **-2.843** | | -4.77 |
| | **-56.48091** | | **-56.22015** | | **-0.26077** | | | |
| | **-210.08268** | | **-209.19181** | | **-0.89088** | | | |
| | (aVDZ) | | | | | | | |
| | -266.32470 | -3.999 | -265.35015 | -1.712 | -0.97455 | -2.287 | | |
| | -56.42639 | | -56.20563 | | -0.22076 | | | |
| | -209.89194 | | -209.14179 | | -0.75015 | | | |
| ***e*** | DEA($H_2O$) | | | | | | | |
| | (aVTZ) | | | | | | | |
| | -440.04111 | -7.707 | -438.22924 | -3.932 | -1.81187 | -3.775 | | -8.07 |
| | -76.34278 | | -76.05929 | | -0.28349 | | | |
| | -363.68605 | | -362.16368 | | -1.52236 | | | |
| | (aVDZ) | | | | | | | |
| | -439.64576 | -6.892 | -438.12497 | -3.969 | -1.52079 | -2.923 | | |
| | -76.27541 | | -76.04065 | | -0.23476 | | | |
| | -363.35936 | | -362.07799 | | -1.28137 | | | |
| ***f*** | DEA($NH_3$) | | | | | | | |
| | (aVTZ) | | | | | | | |
| | -420.17938 | -4.654 | -418.38815 | -1.004 | -1.79123 | -3.650 | | -4.91 |
| | -363.69098 | | -362.16645 | | -1.52453 | | | |
| | -56.48098 | | -56.22010 | | -0.26088 | | | |
| | (aVDZ) | | | | | | | |
| | -419.79773 | -4.078 | -418.28821 | -1.029 | -1.50953 | -3.049 | | |
| | -363.36453 | | -362.08086 | | -1.28368 | | | |
| | -56.42670 | | -56.20571 | | -0.22099 | | | |
| ***g*** | $(MEA)_2$ | | | | | | | |
| | (aVTZ) | | | | | | | |
| | -420.17022 | -4.265 | -418.38312 | -0.227 | -1.78710 | -4.037 | | -4.50 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | -210.08060 | | -209.19066 | | -0.88994 | | | |
| | -210.08282 | | -209.19210 | | -0.89072 | | | |
| | (aVDZ) | | | | | | | |
| | -419.78838 | -3.727 | -418.28327 | -0.249 | -1.50511 | -3.478 | | |
| | -209.89022 | | -209.14075 | | -0.74947 | | | |
| | -209.89222 | | -209.14212 | | -0.75010 | | | |
| | | | | | | | | |
| ***j*** | $NH_3(CO_2)$ | | | | | | | |
| | **(aVQZ)** | | | | | | | |
| | **-244.89007** | **-3.071** | **-243.94617** | **-1.836** | **-0.94389** | **-1.235** | **-3.15** | |
| | **-56.49579** | | **-56.22394** | | **-0.27185** | | | |
| | **-188.38938** | | **-187.71931** | | **-0.67007** | | | |
| | **(aVTZ)** | | | | | | | |
| | **-244.82603** | **-2.940** | **-243.92997** | **-1.817** | **-0.89606** | **-1.123** | | -3.08 |
| | **-56.48070** | | **-56.22031** | | **-0.26039** | | | |
| | **-188.34064** | | **-187.70676** | | **-0.63388** | | | |
| | (aVDZ) | | | | | | | |
| | -244.61657 | -2.608 | -243.86938 | -1.818 | -0.74719 | -0.790 | | |
| | -56.42606 | | -56.20573 | | -0.22033 | | | |
| | -188.18635 | | -187.66075 | | -0.52560 | | | |
| | | | | | | | | |
| ***k*** | $MEA(CO_2)$ | | | | | | | |
| | **(aVQZ)** | | | | | | | |
| | **-398.53313** | **-4.204** | **-396.92645** | **-1.472** | **-1.60668** | **-2.732** | **-4.32** | |
| | **-210.13701** | | **-209.20504** | | **-0.93197** | | | |
| | **-188.38942** | | **-187.71906** | | **-0.67036** | | | |
| | **(aVTZ)** | | | | | | | |
| | **-398.42998** | **-4.022** | **-396.90096** | **-1.450** | **-1.52903** | **-2.572** | | -4.24 |
| | **-210.08258** | | **-209.19202** | | **-0.89056** | | | |
| | **-188.34099** | | **-187.70663** | | **-0.63436** | | | |
| | (aVDZ) | | | | | | | |
| | -398.08434 | -3.513 | -396.80499 | | -1.27934 | -2.046 | | |
| | -209.89167 | | -209.14191 | | -0.74975 | | | |
| | -188.18707 | | -187.66074 | | -0.52633 | | | |
| | | | | | | | | |
| ***l*** | $DEA(CO_2)$ | | | | | | | |
| | (aVTZ) | | | | | | | |
| | -552.03373 | | -549.86991 | 0.363 | -2.16382 | -4.341 | | -4.25 |
| | -188.34145 | | -187.70663 | | -0.63482 | | | |
| | -363.68594 | | -362.16386 | | -1.52208 | | | |
| | (aVDZ) | | | | | | | |
| | -551.55300 | -3.342 | -549.73869 | 0.355 | -1.81431 | -3.697 | | |

| | | |
|---|---|---|
| -188.18840 | -187.66110 | -0.52731 |
| -363.35927 | -362.07816 | -1.28111 |