Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information.

Physical and numerical aspects of sodium ion solvation free energies via the cluster-continuum model.

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Tables mentioned in the main text

Table S1. Calculated $\Delta G_r^*(solv, 298.15\ K)$ according to qRRHO and SMD (1): DLPNO-CCSD(T)/cc-p(wC)VTZ strategy in kcal mol^{-1}.

$Na^+(S)_{n(solv)} + S_{(solv)} \rightarrow Na^+(S)_{n+1(solv)}$	n=4 $\Delta G_r^*(solv, 298.15\ K)$ kcal mol^{-1}	n=5 $\Delta G_r^*(solv, 298.15\ K)$ kcal mol^{-1}
H_2O	6.4	5.2
DMF	5.1	7.7
DMSO	3.2	6.1
EtOH	3.5	2.7
Me_2CO	4.7	5.9
MeCN	2.1	2.0
MeOH	5.2	0.5

Table S2. Calculated $\Delta G_{solv}^*(Na^+(S)_4)$ and $\Delta G_{solv}^*(S)$ according to PCM DLPNO-CCSD(T)/cc-p(wC)VTZ strategy in kcal mol^{-1}.

	$\Delta G_{solv}^*(Na^+(S)_4)$ kcal mol^{-1}	$\Delta G_{solv}^*(S)$ kcal mol^{-1}
$Na^+(H_2O)_4$	-55.6	-5.9
$Na^+(DMF)_4$	-37.3	-6.5
$Na^+(DMSO)_4$	-42.4	-8.4
$Na^+(EtOH)_4$	-44.1	-4.2
$Na^+(Me_2CO)_4$	-36.9	-4.5
$Na^+(MeCN)_4$	-38.4	-6.1
$Na^+(MeOH)_4$	-46.2	-4.2

Table S3. Calculated $\Delta G^{*}_{solv}\left(Na^{+}(S)_4\right)$ and $\Delta G^{*}_{solv}(S)$ according to SMD (1): SMD DLPNO-CCSD(T)/cc-p(wC)TZ strategy in kcal mol^{-1}.

	$\Delta G^{*}_{solv}\left(Na^{+}(S)_4\right)$ kcal mol^{-1}	$\Delta G^{*}_{solv}(S)$ kcal mol^{-1}
$Na^{+}(H_2O)_4$	-58.5	-7.3
$Na^{+}(DMF)_4$	-38.7	-6.2
$Na^{+}(DMSO)_4$	-40.8	-6.9
$Na^{+}(EtOH)_4$	-51.1	-5.7
$Na^{+}(Me_2CO)_4$	-43.2	-5.6
$Na^{+}(MeCN)_4$	-44.5	-6.8
$Na^{+}(MeOH)_4$	-50.0	-4.8

Table S4. Calculated $\Delta G^{*}_{solv}\left(Na^{+}(S)_4\right)$ ***and*** $\Delta G^{*}_{solv}(S)$ ***according to SMD (2): PBE0/def2-tzvp strategy in kcal mol^{-1}.***

	$\Delta G^{*}_{solv}\left(Na^{+}(S)_4\right)$ kcal mol^{-1}	$\Delta G^{*}_{solv}(S)$ kcal mol^{-1}
$Na^{+}(H_2O)_4$	-57.0	-8.2
$Na^{+}(DMF)_4$	-39.4	-6.7
$Na^{+}(DMSO)_4$	-41.2	-7.4
$Na^{+}(EtOH)_4$	-51.8	-6.1
$Na^{+}(Me_2CO)_4$	-43.9	-6.4
$Na^{+}(MeCN)_4$	-44.5	-6.8
$Na^{+}(MeOH)_4$	-50.7	-5.2

Table S5. Calculated $\Delta G^{*}_{solv}\left(Na^{+}(S)_4\right)$ ***and*** $\Delta G^{*}_{solv}(S)$ ***according to SMD (3): B3LYP/6-31G(d) strategy in kcal mol^{-1}.***

	$\Delta G^{*}_{solv}\left(Na^{+}(S)_4\right)$ kcal mol^{-1}	$\Delta G^{*}_{solv}(S)$ kcal mol^{-1}
$Na^{+}(H_2O)_4$	-59.7	-8.2
$Na^{+}(DMF)_4$	-38.0	-5.7
$Na^{+}(DMSO)_4$	-40.2	-6.6
$Na^{+}(EtOH)_4$	-51.6	-5.8
$Na^{+}(Me_2CO)_4$	-43.0	-5.5
$Na^{+}(MeCN)_4$	-43.3	-6.0
$Na^{+}(MeOH)_4$	-50.4	-5.1

Table S6. $nRT\ln[S]$ ***terms for*** $Na^+(S)_4$ ***in kcal mol^{-1}.***

	$nRT\ln[S]$ kcal mol^{-1}
$Na^+(H_2O)_4$	14.268
$Na^+(DMF)_4$	6.064
$Na^+(DMSO)_4$	6.256
$Na^+(EtOH)_4$	6.72
$Na^+(Me_2CO)_4$	6.168
$Na^+(MeCN)_4$	6.968
$Na^+(MeOH)_4$	7.58

Tables forming the basis of Figures 1 – 5 in the main text

Table S7. Deviations of our predicted gas-phase DLPNO-CCSD(T) clusterization energies $^{\Delta E_{clust}(Na^+(S)_4)}$ obtained with cc-p(wC)VTZ and cc-p(wC)QZ basis sets from their CBS(TZ/QZ) counterparts in kcal mol^{-1} (Figure 1).

	TZ[a]	QZ[b]
$Na^+(H_2O)_4$	-8.7	-3.2
$Na^+(DMF)_4$	-4.6	-1.7
$Na^+(DMSO)_4$	-11.5	-4.2
$Na^+(EtOH)_4$	-6.5	-2.4
$Na^+(Me_2CO)_4$	-3.8	-1.4
$Na^+(MeCN)_4$	-2.7	-1.0
$Na^+(MeOH)_4$	-6.7	-2.5

[a] $\Delta E_{clust}\left(Na^+(S)_4\right)(TZ) - \Delta E_{clust}\left(Na^+(S)_4\right)(CBS)$

[b] $\Delta E_{clust}\left(Na^+(S)_4\right)(QZ) - \Delta E_{clust}\left(Na^+(S)_4\right)(CBS)$

Table S8. Individual contributions to $^{\Delta E_{clust}(Na^+(S)_4)}$ calculated via eqn. (2): $^{\Delta E_{CV}}$, $^{\Delta E_{IT}}$, $^{\Delta E_{PNO}}$, and $^{\Delta E_{SR}}$ in kcal mol^{-1} (Figure 2).

	ΔE_{CV} kcal mol^{-1}	ΔE_{PNO} kcal mol^{-1}	ΔE_{IT} kcal mol^{-1}	ΔE_{SR} kcal mol^{-1}
$Na^+(H_2O)_4$	-0.1	-0.1	0.0	0.1
$Na^+(DMF)_4$	0.0	-0.1	0.0	0.0
$Na^+(DMSO)_4$	0.0	0.3	0.1	0.0
$Na^+(EtOH)_4$	0.1	-0.2	0.0	0.0
$Na^+(Me_2CO)_4$	0.0	0.1	0.1	0.0
$Na^+(MeCN)_4$	0.0	0.7	0.0	0.0
$Na^+(MeOH)_4$	0.0	0.0	0.0	0.1

Table S9. $\Delta G^{*}_{clust} - \Delta E_{clust}$ ***contributions to the Gibbs free energies of*** $Na^{+}(S)_4$ ***cluster formation in gas-phase as predicted by HO, qRRHO and HO(100) models, see Section 2.3 (Figure 3).***

	$\Delta G^{*}_{clust} - \Delta E_{clust}$ (HO)[a] kcal mol^{-1}	$\Delta G^{*}_{clust} - \Delta E_{clust}$ (qRRHO)[a] kcal mol^{-1}	$\Delta G^{*}_{clust} - \Delta E_{clust}$ (HO(100))[a] kcal mol^{-1}
$Na^{+}(H_2O)_4$	23.80	27.21	28.00
$Na^{+}(DMF)_4$	28.32	37.86	41.69
$Na^{+}(DMSO)_4$	33.29	39.81	41.23
$Na^{+}(EtOH)_4$	32.16	37.84	38.47
$Na^{+}(Me_2CO)_4$	30.36	36.27	37.31
$Na^{+}(MeCN)_4$	21.38	29.60	32.51
$Na^{+}(MeOH)_4$	28.20	33.20	33.90
[a] See Section 2.3 in the main text for details.			

Table S10. $\Delta\Delta G^{*}_{solv} = \Delta G^{*}_{solv}\left(Na^{+}(S)_n\right) - n\Delta G^{*}_{solv}(S)$ ***contributions to the Gibbs free energies of solvation as calculated with PCM DLPNO-CCSD(T)/cc-p(wC)VTZ, SMD (1): SMD DLPNO-CCSD(T)/cc-p(wC)TZ, SMD (2): PBE0/def2-tzvp, SMD (3): B3LYP/6-31G(d). (Figure 4).***

	$\Delta\Delta G^{*}_{solv}$ PCM[a] kcal mol^{-1}	$\Delta\Delta G^{*}_{solv}$ SMD (1)[b] kcal mol^{-1}	$\Delta\Delta G^{*}_{solv}$ SMD (2)[c] kcal mol^{-1}	$\Delta\Delta G^{*}_{solv}$ SMD (3)[d] kcal mol^{-1}
$Na^{+}(H_2O)_4$	-25.13	-29.48	-26.74	-26.89
$Na^{+}(DMF)_4$	-11.27	-13.99	-12.51	-15.16
$Na^{+}(DMSO)_4$	-8.83	-13.05	-11.47	-13.79
$Na^{+}(EtOH)_4$	-27.21	-28.31	-27.27	-28.25
$Na^{+}(Me_2CO)_4$	-18.95	-20.67	-18.35	-20.92
$Na^{+}(MeCN)_4$	-13.90	-18.82	-17.30	-19.39
$Na^{+}(MeOH)_4$	-29.45	-30.96	-29.96	-30.01

[a] PCM DLPNO-CCSD(T)/cc-p(wC)VTZ; [b] SMD (1): SMD DLPNO-CCSD(T)/cc-p(wC)TZ; [c] SMD (2): PBE0/def2-tzvp; [d] SMD (3): B3LYP/6-31G(d).

Table S11. Experimental and predicted solvation free energies $\Delta G^*_{solv}(Na^+)$ ***in kcal mol^{-1} (Figure 5).***

	$\Delta G^*_{solv}(Na^+)$ Theor. kcal mol^{-1}	$\Delta G^*_{solv}(Na^+)$ Expt. kcal mol^{-1}
$Na^+(H_2O)_4$	-92.0±2.6	-91.6±1.4
$Na^+(DMF)_4$	-93.0±3.8	-94.2±1.5
$Na^+(DMSO)_4$	-95.3±3.0	-94.7±1.5
$Na^+(EtOH)_4$	-86.1±1.1	-88.1±1.5
$Na^+(Me_2CO)_4$	-86.6±2.0	-89.3±1.5
$Na^+(MeCN)_4$	-91.8±2.5	-88.8±1.5
$Na^+(MeOH)_4$	-90.0±1.5	-90.0±1.5

Cartesian Coordinates (Å) and Absolute Energies (Hartree) of All Species Studied in Present Work

WATER SOLVENT

H_2O

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Charge of molecule: 0
Multiplicity: 1
E(HF/CC-PVTZ) = -76.0570175
E(DLPNO-CCSD(T)/CC-PVTZ) = -76.3321042493
T1 (CC-PVTZ)= 0.006534381
T2 (CC-PVTZ)= 0.033817
E(HF/CC-PVQZ) = -76.06468126
E(DLPNO-CCSD(T)/CC-PVQZ) = -76.3597135304
E(HF/DZ-CORE) = -76.02701699
E(DLPNO-CCSD(T)/DZ-CORE) = -76.2781368417
E(HF/DZ-CORE (FC)) = -76.02701699
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -
76.2473286087
E(HF/TZ-CORE) = -76.05713487
E(DLPNO-CCSD(T)/TZ-CORE) = -76.389766942
E(HF/TZ-CORE (FC)) = -76.05713487
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -
76.3369267916
E(HF/TZ-IT) = -76.0570175
E(DLPNO-CCSD(T)/TZ-IT) = -76.332369115
E(IT_EFFECT) = -0.000264865653989
T1 (CC-PVQZ)= 0.007300434
T2 (CC-PVQZ)= 0.047392
E(HF/TZ-DKH) = -76.10868353
E(DLPNO-CCSDT/TZ-DKH) = -76.3839342933
E(HF/CBS) = -76.0691045022
E(DLPNO-CCSD(T)/CBS) = -76.3756485987
E(DLPNO_TPNO/CC-PVTZ)) = -76.3320787505
E(CV correction (DZ)) = -0.03080823301
E(CV correction (TZ)) = -0.052840150347
E(CV correction (CBS)) = -0.0605934996351
E(TPNO_EFFECT) = 2.54987990047e-05
E(DKH correction) = -0.051830043987
E(HF/TZ-SMD) = -76.07004293
E(DLPNO-CCSDT/TZ-SMD) = -76.3436548799
dG(solv_DLPNO_SMD) = -0.011576129383
E(HF/TZ-PCM) = -76.06744103
E(DLPNO-CCSDT/TZ-PCM) = -76.341538077624
dG(solv_DLPNO_PCM) = -0.00945933
E(PBE0/TZ-GAS) = -76.3774806731
E(PBE0/TZ-SMD) = -76.3905431037
dG(solv_PBE0_SMD) = -0.013062430569
E(B3LYP/6-31G(d)-GAS) = -76.369811352494
E(B3LYP/6-31G(d)-SMD) = -76.382873211845
dG(solv_B3LYP_6-31G(d)_SMD) = -0.01306186
dGcorr (HO): 0.0034854000
dGcorr(HO(100)): 0.0034854000
dGcorr(qRRHO): 0.0038502200
```

O	0.000000	0.000000	-0.389133
H	0.000000	0.761558	0.194567
H	0.000000	-0.761558	0.194567

$Na^+(H_2O)_4$

```
Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -466.03831273
E(DLPNO-CCSD(T)/CC-PVTZ) = -467.400922589
T1 (CC-PVTZ)= 0.006984012
T2 (CC-PVTZ)= 0.034036
E(HF/CC-PVQZ) = -466.06339321
E(DLPNO-CCSD(T)/CC-PVQZ) = -467.54161053
E(HF/DZ-CORE) = -465.93669189
E(DLPNO-CCSD(T)/DZ-CORE) = -467.05934391
E(HF/DZ-CORE (FC)) = -465.93669189
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -
466.936014006
E(HF/TZ-CORE) = -466.03879915
E(DLPNO-CCSD(T)/TZ-CORE) = -467.631295155
E(HF/TZ-CORE (FC)) = -466.03879915
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -
467.419833539
E(HF/TZ-IT) = -466.03831273
E(DLPNO-CCSD(T)/TZ-IT) = -467.402112728
E(IT_EFFECT) = -0.001190138629
T1 (CC-PVQZ)= 0.006962961
T2 (CC-PVQZ)= 0.046432
E(HF/TZ-DKH) = -466.45371407
E(DLPNO-CCSDT/TZ-DKH) = -467.81725085
E(HF/CBS) = -466.077868747
E(DLPNO-CCSD(T)/CBS) = -467.622810469
E(DLPNO_TPNO/CC-PVTZ)) = -467.400956233
E(CV correction (DZ)) = -0.123329904188
E(CV correction (TZ)) = -0.211461616604
E(CV correction (CBS)) = -0.24247643657
E(TPNO_EFFECT) = -3.36432490258e-05
E(DKH correction) = -0.416328260396
E(HF/TZ-SMD) = -466.13281539
E(DLPNO-CCSDT/TZ-SMD) = -467.494261458477
dG(solv_DLPNO_SMD) = -0.09330523
E(HF/TZ-PCM) = -466.12758768
E(DLPNO-CCSDT/TZ-PCM) = -467.489564947649
dG(solv_DLPNO_PCM) = -0.08860871
E(PBE0/TZ-GAS) = -467.630643024
E(PBE0/TZ-SMD) = -467.725511023
dG(solv_PBE0_SMD) = -0.094867999512
E(B3LYP/6-31G(d)-GAS) = -467.6860105045
E(B3LYP/6-31G(d)-SMD) = -467.781107116604
dG(solv_B3LYP_6-31G(d)_SMD) = -0.09509661
dGcorr (HO): 0.0494916200
dGcorr(HO(100)): 0.0561849900
dGcorr(qRRHO): 0.0563759400
```

Na	-0.016328	0.037338	-0.013768
O	-1.715947	-1.036816	1.099072
H	-2.479359	-1.473431	0.711417
H	-1.838201	-1.105244	2.049960
O	1.253070	1.432453	1.291603
H	1.956411	1.179319	1.895584
H	1.212235	2.391794	1.334109
O	1.508503	-1.553588	-0.651162
H	1.379449	-2.505647	-0.623183
H	2.388134	-1.425616	-1.016525
O	-1.041631	1.166947	-1.732591
H	-0.755922	1.207664	-2.649492
H	-1.850415	1.684826	-1.695023

$Na^+(H_2O)_5$

Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -542.11181704
E(DLPNO-CCSD(T)/CC-PVTZ) = -543.755589378
T1 (CC-PVTZ)= 0.007191221
T2 (CC-PVTZ)= 0.036204
E(HF/CC-PVQZ) = -542.14277105
E(DLPNO-CCSD(T)/CC-PVQZ) = -543.921429404
E(HF/DZ-CORE) = -541.98470357
E(DLPNO-CCSD(T)/DZ-CORE) = -543.364305479
E(HF/DZ-CORE (FC)) = -541.98470357
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -543.210165414
E(HF/TZ-CORE) = -542.11243899
E(DLPNO-CCSD(T)/TZ-CORE) = -544.043442239
E(HF/TZ-CORE (FC)) = -542.11243899
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -543.779209989
E(HF/TZ-IT) = -542.11181704
E(DLPNO-CCSD(T)/TZ-IT) = -543.757078385
E(IT_EFFECT) = -0.001489006866
T1 (CC-PVQZ)= 0.007214891
T2 (CC-PVQZ)= 0.046707
E(HF/TZ-DKH) = -542.57887114
E(DLPNO-CCSDT/TZ-DKH) = -544.223731075
E(HF/CBS) = -542.160636574
E(DLPNO-CCSD(T)/CBS) = -544.017146208
E(DLPNO_TPNO/CC-PVTZ)) = -543.755579587
E(CV correction (DZ)) = -0.154140065209
E(CV correction (TZ)) = -0.26423224934
E(CV correction (CBS)) = -0.30297527585
E(TPNO_EFFECT) = 9.79058097528e-06
E(DKH correction) = -0.468141697679
E(HF/TZ-SMD) = -542.20516333
E(DLPNO-CCSDT/TZ-SMD) = -543.847190455258
dG(solv_DLPNO_SMD) = -0.09161087
E(HF/TZ-PCM) = -542.20002971
E(DLPNO-CCSDT/TZ-PCM) = -543.842899667029
dG(solv_DLPNO_PCM) = -0.08732008
E(PBE0/TZ-GAS) = -544.029425215
E(PBE0/TZ-SMD) = -544.123032618
dG(solv_PBE0_SMD) = -0.0936074023409
E(B3LYP/6-31G(d)-GAS) = -544.0802297869
E(B3LYP/6-31G(d)-SMD) = -544.174703791596
dG(solv_B3LYP_6-31G(d)_SMD) = -0.09447400
dGcorr (HO): 0.0715980200
dGcorr(HO(100)): 0.0780541600
dGcorr(qRRHO): 0.0787677100

Na	0.010623	-0.005966	-0.002373
O	2.252916	-0.491328	0.788058
H	2.883281	0.199101	1.012897
H	2.450195	-1.219674	1.384118
O	-0.025309	2.308140	-0.035549
H	-0.303725	2.892915	0.674174
H	0.258196	2.884675	-0.749981
O	-1.135552	-0.733247	1.848579
H	-1.139824	-0.925530	2.788351
H	-2.017612	-0.931901	1.518016
O	1.154880	-0.779350	-1.834912
H	2.034956	-0.988410	-1.505848
H	1.147956	-0.996450	-2.769278
O	-2.245272	-0.488754	-0.765508
H	-2.471063	-1.227001	-1.338809
H	-2.854357	0.215526	-1.005717

$Na^+(H_2O)_6$

Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -618.1893926
E(DLPNO-CCSD(T)/CC-PVTZ) = -620.114632726
T1 (CC-PVTZ)= 0.007205161
T2 (CC-PVTZ)= 0.036878
E(HF/CC-PVQZ) = -618.22693071
E(DLPNO-CCSD(T)/CC-PVQZ) = -620.307486269
E(HF/DZ-CORE) = -618.0365152
E(DLPNO-CCSD(T)/DZ-CORE) = -619.672014417
E(HF/DZ-CORE (FC)) = -618.0365152
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -619.487030289
E(HF/TZ-CORE) = -618.19008658
E(DLPNO-CCSD(T)/TZ-CORE) = -620.459998946
E(HF/TZ-CORE (FC)) = -618.19008658
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -620.142906751
E(HF/TZ-IT) = -618.1893926
E(DLPNO-CCSD(T)/TZ-IT) = -620.116438808
E(IT_EFFECT) = -0.00180608160395
T1 (CC-PVQZ)= 0.007288495
T2 (CC-PVQZ)= 0.046877
E(HF/TZ-DKH) = -618.70804978
E(DLPNO-CCSDT/TZ-DKH) = -620.634548778
E(HF/CBS) = -618.248596336
E(DLPNO-CCSD(T)/CBS) = -620.418794288
E(DLPNO_TPNO/CC-PVTZ)) = -620.114458875
E(CV correction (DZ)) = -0.184984128262
E(CV correction (TZ)) = -0.317092194452
E(CV correction (CBS)) = -0.363582927205
E(TPNO_EFFECT) = 0.000173851262048
E(DKH correction) = -0.519916051863
E(HF/TZ-SMD) = -618.27952114
E(DLPNO-CCSDT/TZ-SMD) = -620.202912295076
dG(solv_DLPNO_SMD) = -0.08845342
E(HF/TZ-PCM) = -618.27416542
E(DLPNO-CCSDT/TZ-PCM) = -620.19814543526
dG(solv_DLPNO_PCM) = -0.08368656
E(PBE0/TZ-GAS) = -620.436956957
E(PBE0/TZ-SMD) = -620.527801227
dG(solv_PBE0_SMD) = -0.0908442691709
E(B3LYP/6-31G(d)-GAS) = -620.4843765823
E(B3LYP/6-31G(d)-SMD) = -620.576583809518
dG(solv_B3LYP_6-31G(d)_SMD) = -0.09220723
dGcorr (HO): 0.0980569700
dGcorr(HO(100)): 0.1034067500
dGcorr(qRRHO): 0.1050358400

Na	0.020992	-0.043574	-0.019662
O	-0.748371	-2.048346	3.411597
H	-0.185905	-2.679541	3.871689
H	-1.551832	-1.979055	3.937067
O	0.375649	0.282780	2.215074
H	0.064614	-0.403852	2.824212
H	0.771147	0.972977	2.750456
O	0.715732	2.138135	-3.365945
H	1.137832	3.002718	-3.394197
H	0.506948	1.916481	-4.279021
O	1.682616	0.138562	-1.577805
H	1.560131	0.778207	-2.295530
H	2.540089	-0.269576	-1.710533
O	-1.111159	1.504637	-1.263022
H	-1.966686	1.933625	-1.204317
H	-0.667051	1.866821	-2.044440
O	-0.901957	-2.053275	0.558871
H	-1.288267	-2.790599	0.082957
H	-0.954521	-2.267126	1.502552

DMF SOLVENT

DMF

```
Charge of molecule: 0
Multiplicity: 1
E(HF/CC-PVTZ) = -247.08248341
E(DLPNO-CCSD(T)/CC-PVTZ) = -248.104719471
T1 (CC-PVTZ)= 0.013200931
T2 (CC-PVTZ)= 0.043975
E(HF/CC-PVQZ) = -247.10031392
E(DLPNO-CCSD(T)/CC-PVQZ) = -248.181396791
E(HF/DZ-CORE) = -247.01198611
E(DLPNO-CCSD(T)/DZ-CORE) = -248.019198661
E(HF/DZ-CORE (FC)) = -247.01198611
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -
247.866554582
E(HF/TZ-CORE) = -247.08413006
E(DLPNO-CCSD(T)/TZ-CORE) = -248.368529938
E(HF/TZ-CORE (FC)) = -247.08413006
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -
248.120289379
E(HF/TZ-IT) = -247.08248341
E(DLPNO-CCSD(T)/TZ-IT) = -248.106551543
E(IT_EFFECT) = -0.00183207203301
T1 (CC-PVQZ)= 0.012945859
T2 (CC-PVQZ)= 0.044048
E(HF/TZ-DKH) = -247.20681849
E(DLPNO-CCSDT/TZ-DKH) = -248.229492216
E(HF/CBS) = -247.110605039
E(DLPNO-CCSD(T)/CBS) = -248.225652138
E(DLPNO_TPNO/CC-PVTZ)) = -248.105101475
E(CV correction (DZ)) = -0.152644078705
E(CV correction (TZ)) = -0.248240558569
E(CV correction (CBS)) = -0.2818823378
E(TPNO_EFFECT) = -0.000382003458014
E(DKH correction) = -0.124772745147
E(HF/TZ-SMD) = -247.09414119
E(DLPNO-CCSDT/TZ-SMD) = -248.115022352744
dG(solv_DLPNO_SMD) = -0.00992088
E(HF/TZ-PCM) = -247.09530481
E(DLPNO-CCSDT/TZ-PCM) = -248.115529931589
dG(solv_DLPNO_PCM) = -0.01042846
E(PBE0/TZ-GAS) = -248.320607365
E(PBE0/TZ-SMD) = -248.331309944
dG(solv_PBE0_SMD) = -0.01070257883
E(B3LYP/6-31G(d)-GAS) = -248.359677240649
E(B3LYP/6-31G(d)-SMD) = -248.368780512721
dG(solv_B3LYP_6-31G(d)_SMD) = -0.00910327
dGcorr (HO): 0.0717141800
dGcorr(HO(100)): 0.0717141800
dGcorr(qRRHO): 0.0735658700
```

H	2.256401	0.529485	0.886781
O	-1.851931	0.071465	0.000352
C	-0.776279	0.626023	-0.000291
H	-0.675872	1.728030	0.000386
N	0.428955	0.011916	-0.000127
C	0.512705	-1.424829	-0.000036
H	1.044767	-1.781534	-0.887686
H	-0.499506	-1.824769	-0.000150
H	1.044543	-1.781441	0.887785
C	1.655608	0.757952	0.000021
H	1.434191	1.826039	0.000044
H	2.256569	0.529557	-0.886643

$Na^+(DMF)_4$

```
Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -1150.18260179
E(DLPNO-CCSD(T)/CC-PVTZ) = -1154.53390938
T1 (CC-PVTZ)= 0.012806249
T2 (CC-PVTZ)= 0.040141
E(HF/CC-PVQZ) = -1150.25081579
E(DLPNO-CCSD(T)/CC-PVQZ) = -1154.87501421
E(HF/DZ-CORE) = -1149.9119939
E(DLPNO-CCSD(T)/DZ-CORE) = -1154.05413849
E(HF/DZ-CORE (FC)) = -1149.9119939
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -
1153.44338063
E(HF/TZ-CORE) = -1150.18895384
E(DLPNO-CCSD(T)/TZ-CORE) = -1155.58843643
E(HF/TZ-CORE (FC)) = -1150.18895384
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -
1154.59543868
E(HF/TZ-IT) = -1150.18260179
E(DLPNO-CCSD(T)/TZ-IT) = -1154.54125039
E(IT_EFFECT) = -0.00734100985892
T1 (CC-PVQZ)= 0.012554660
T2 (CC-PVQZ)= 0.042907
E(HF/TZ-DKH) = -1150.88873318
E(DLPNO-CCSDT/TZ-DKH) = -1155.24206534
E(HF/CBS) = -1150.29018642
E(DLPNO-CCSD(T)/CBS) = -1155.07188745
E(DLPNO_TPNO/CC-PVTZ)) = -1154.53552908
E(CV correction (DZ)) = -0.610757853006
E(CV correction (TZ)) = -0.992997749687
E(CV correction (CBS)) = -1.12751347909
E(TPNO_EFFECT) = -0.00161969400892
E(DKH correction) = -0.708155961091
E(HF/TZ-SMD) = -1150.2470624
E(DLPNO-CCSDT/TZ-SMD) = -1154.59741675512
dG(solv_DLPNO_SMD) = -0.06188768
E(HF/TZ-PCM) = -1150.24516493
E(DLPNO-CCSDT/TZ-PCM) = -1154.59508924057
dG(solv_DLPNO_PCM) = -0.05956016
E(PBE0/TZ-GAS) = -1155.47217426
E(PBE0/TZ-SMD) = -1155.53492519
dG(solv_PBE0_SMD) = -0.0627509283811
E(B3LYP/6-31G(d)-GAS) = -1155.6766423000
E(B3LYP/6-31G(d)-SMD) = -1155.73721201165
dG(solv_B3LYP_6-31G(d)_SMD) = -0.06056971
dGcorr (HO): 0.3296042000
dGcorr(HO(100)): 0.3509147300
dGcorr(qRRHO): 0.3522221600
```

Na	0.426535	-0.059134	-0.095805
H	-4.551360	3.379651	1.450976
O	-0.736002	1.751616	0.661697
C	-1.912092	2.012163	0.431377
H	-2.539746	1.343977	-0.179012
N	-2.560386	3.092808	0.869223
C	-1.896249	4.077233	1.690182
H	-1.882885	5.046924	1.185345
H	-0.876596	3.747812	1.875000
H	-2.420658	4.189864	2.642425
C	-3.945762	3.324543	0.542492
H	-4.319004	2.510000	-0.077852
H	-4.060055	4.263135	-0.006357
H	-3.912910	-4.316572	-1.754588
O	-1.298780	-1.047310	-1.207746
C	-1.620861	-2.230116	-1.226400
H	-1.159662	-2.962876	-0.545085
N	-2.532281	-2.767975	-2.038253
C	-3.230687	-1.960717	-3.010402

H	-3.064157	-2.354723	-4.016061
H	-2.854424	-0.942155	-2.953677
H	-4.305186	-1.967430	-2.808802
C	-2.854105	-4.172758	-1.985637
H	-2.259526	-4.658360	-1.212070
H	-2.641632	-4.652378	-2.944759
H	2.015196	-4.782681	4.027245
O	1.015264	-1.821011	1.192306
C	1.416189	-2.248228	2.268643
H	1.270933	-1.685804	3.204307
N	2.055609	-3.403908	2.451484
C	2.352941	-4.274496	1.338920
H	3.429489	-4.451955	1.277836
H	2.011984	-3.800157	0.421845
H	1.849925	-5.237126	1.464094
C	2.482248	-3.830578	3.762163
H	2.198703	-3.084374	4.503977
H	3.567514	-3.957861	3.789746
H	3.776686	4.579788	-2.467223
O	2.132514	0.941222	-1.083221
C	3.000457	1.685224	-1.518020
H	3.804982	1.308158	-2.168497
N	3.094562	2.995049	-1.280345
C	2.129539	3.678938	-0.452312
H	2.619843	4.100364	0.429762
H	1.358425	2.978749	-0.138314
H	1.669695	4.496334	-1.014319
C	4.170422	3.782200	-1.831696
H	4.822713	3.148045	-2.431558
H	4.762640	4.236886	-1.033032

$Na^+(DMF)_5$

```
Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -1397.27889036
E(DLPNO-CCSD(T)/CC-PVTZ) = -1402.66431422
T1 (CC-PVTZ)= 0.012848933
T2 (CC-PVTZ)= 0.040539
E(HF/CC-PVQZ) = -1397.36338493
E(DLPNO-CCSD(T)/CC-PVQZ) = -1403.08025531
E(HF/DZ-CORE) = -1396.94181822
E(DLPNO-CCSD(T)/DZ-CORE) = -1402.10261658
E(HF/DZ-CORE (FC)) = -1396.94181822
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -
1401.33922648
E(HF/TZ-CORE) = -1397.28684973
E(DLPNO-CCSD(T)/TZ-CORE) = -1403.98273747
E(HF/TZ-CORE (FC)) = -1397.28684973
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -
1402.74165595
E(HF/TZ-IT) = -1397.27889036
E(DLPNO-CCSD(T)/TZ-IT) = -1402.67346914
E(IT_EFFECT) = -0.00915492059198
T1 (CC-PVQZ)= 0.012588602
T2 (CC-PVQZ)= 0.041346
E(HF/TZ-DKH) = -1398.10935807
E(DLPNO-CCSDT/TZ-DKH) = -1403.49724737
E(HF/CBS) = -1397.41215211
E(DLPNO-CCSD(T)/CBS) = -1403.32032132
E(DLPNO_TPNO/CC-PVTZ)) = -1402.6668466
E(CV correction (DZ)) = -0.763390100095
E(CV correction (TZ)) = -1.24108151401
E(CV correction (CBS)) = -1.40918800821
E(TPNO_EFFECT) = -0.00253238350297
E(DKH correction) = -0.832933156981
E(HF/TZ-SMD) = -1397.34252758
E(DLPNO-CCSDT/TZ-SMD) = -1402.72836554019
dG(solv_DLPNO_SMD) = -0.06151894
E(HF/TZ-PCM) = -1397.34196787
E(DLPNO-CCSDT/TZ-PCM) = -1402.72698275993
dG(solv_DLPNO_PCM) = -0.06013616
E(PBE0/TZ-GAS) = -1403.82292505
E(PBE0/TZ-SMD) = -1403.88556669
dG(solv_PBE0_SMD) = -0.0626416372841
E(B3LYP/6-31G(d)-GAS) = -1404.0562382096
E(B3LYP/6-31G(d)-SMD) = -1404.11640643297
dG(solv_B3LYP_6-31G(d)_SMD) = -0.06016822
dGcorr (HO): 0.4240333400
dGcorr(HO(100)): 0.4452448000
dGcorr(qRRHO): 0.4496514900
```

Na	-0.217734	-0.480047	0.112400
H	1.368159	1.886608	-5.464619
O	-0.183023	-0.303064	-2.205792
C	0.682875	0.272916	-2.851363
H	1.527494	0.777079	-2.356516
N	0.715194	0.361452	-4.185565
C	-0.311114	-0.251418	-4.992723
H	0.131129	-0.969584	-5.688200
H	-1.006339	-0.766760	-4.333597
H	-0.846899	0.506148	-5.571559
C	1.772086	1.063351	-4.868784
H	2.471794	1.471450	-4.139511
H	2.315931	0.389289	-5.536384
H	-3.838804	-1.364169	-3.835113
O	-1.944015	-2.027530	-0.148207
C	-2.661001	-2.307874	-1.099298
H	-2.741808	-3.341859	-1.471986
N	-3.422849	-1.452092	-1.784159
C	-3.461268	-0.048429	-1.448703
H	-4.498401	0.294343	-1.438793
H	-3.019384	0.106013	-0.467308
H	-2.898519	0.536899	-2.180886
C	-4.180854	-1.879450	-2.932501
H	-4.059431	-2.952731	-3.078058
H	-5.243539	-1.662755	-2.795581
H	5.197117	1.023725	2.742831
O	1.849979	0.721670	0.180789
C	2.747865	0.304529	0.905936
H	2.623067	-0.617297	1.492428
N	3.937164	0.891523	1.074277
C	4.271463	2.114038	0.386441
H	5.138771	1.963134	-0.262214
H	3.418085	2.419997	-0.214532
H	4.512866	2.901483	1.105627
C	4.936195	0.323188	1.944767
H	4.551843	-0.592052	2.394450
H	5.844886	0.083194	1.385869
H	-0.868701	5.038956	2.950375
O	-1.329739	1.383240	0.890292
C	-0.823007	2.469413	1.138460
H	0.248637	2.655469	0.964396
N	-1.472911	3.527798	1.632393
C	-2.883587	3.460725	1.929186
H	-3.435943	4.183654	1.322640
H	-3.237964	2.456156	1.710653
H	-3.059308	3.687527	2.983989
C	-0.795650	4.772813	1.892234
H	0.257647	4.680146	1.627475
H	-1.234468	5.582622	1.302679
H	-1.028285	-4.429666	4.704417
O	0.643331	-1.863731	1.795320
C	-0.032057	-2.802796	2.207406
H	-0.939808	-3.123172	1.676585
N	0.233557	-3.518722	3.303302
C	1.378862	-3.228166	4.129445
H	2.068700	-4.076615	4.141776
H	1.885636	-2.354246	3.727118
H	1.062610	-3.024223	5.155815

C	-0.617219	-4.610520	3.707418
H	-1.442156	-4.712133	3.002794
H	-0.057160	-5.549443	3.729970

$Na^{+}(DMF)_6$

```
Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -1644.35703491
E(DLPNO-CCSD(T)/CC-PVTZ) = -1650.78970252
T1 (CC-PVTZ)= 0.012885242
T2 (CC-PVTZ)= 0.042640
E(HF/CC-PVQZ) = -1644.45779767
E(DLPNO-CCSD(T)/CC-PVQZ) = -1651.28082944
E(HF/DZ-CORE) = -1643.95339297
E(DLPNO-CCSD(T)/DZ-CORE) = -1650.14532557
E(HF/DZ-CORE (FC)) = -1643.95339297
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -
1649.22920352
E(HF/TZ-CORE) = -1644.36661399
E(DLPNO-CCSD(T)/TZ-CORE) = -1652.37066806
E(HF/TZ-CORE (FC)) = -1644.36661399
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -
1650.88150253
E(HF/TZ-IT) = -1644.35703491
E(DLPNO-CCSD(T)/TZ-IT) = -1650.80074949
E(IT_EFFECT) = -0.0110469675221
T1 (CC-PVQZ)= 0.012689601
T2 (CC-PVQZ)= 0.047986
E(HF/TZ-DKH) = -1645.31182071
E(DLPNO-CCSDT/TZ-DKH) = -1651.74738868
E(HF/CBS) = -1644.51595425
E(DLPNO-CCSD(T)/CBS) = -1651.56428995
E(DLPNO_TPNO/CC-PVTZ)) = -1650.79182184
E(CV correction (DZ)) = -0.916122049707
E(CV correction (TZ)) = -1.48916552992
E(CV correction (CBS)) = -1.6908277907
E(TPNO_EFFECT) = -0.00211931638819
E(DKH correction) = -0.957686160508
E(HF/TZ-SMD) = -1644.42297947
E(DLPNO-CCSDT/TZ-SMD) = -1650.85430319923
dG(solv_DLPNO_SMD) = -0.06248136
E(HF/TZ-PCM) = -1644.42428662
E(DLPNO-CCSDT/TZ-PCM) = -1650.85431906725
dG(solv_DLPNO_PCM) = -0.06249723
E(PBE0/TZ-GAS) = -1652.09639188
E(PBE0/TZ-SMD) = -1652.16021229
dG(solv_PBE0_SMD) = -0.0638204126672
E(B3LYP/6-31G(d)-GAS) = -1652.4221956996
E(B3LYP/6-31G(d)-SMD) = -1652.48293461671
dG(solv_B3LYP_6-31G(d)_SMD) = -0.06073892
dGcorr (HO): 0.5181625300
dGcorr(HO(100)): 0.5400003000
dGcorr(qRRHO): 0.5468246700
```

Na	0.202885	0.059434	0.060936
H	4.339395	2.188103	-3.107569
O	2.554261	0.189558	0.149115
C	3.442127	0.470198	-0.642431
H	4.183977	-0.279679	-0.963813
N	3.645466	1.665625	-1.202354
C	2.784401	2.787396	-0.914657
H	3.371690	3.612823	-0.502417
H	2.019201	2.489573	-0.202734
H	2.297189	3.130686	-1.831191
C	4.725350	1.882772	-2.130499
H	5.298954	0.964170	-2.253823
H	5.395673	2.666568	-1.767046
H	1.762885	-5.517745	1.941638
O	0.140534	-2.285829	-0.277451
C	0.135166	-3.319698	0.373875
H	-0.636686	-4.092867	0.215034
N	1.013296	-3.665938	1.317451
C	2.120329	-2.808641	1.671506
H	1.988186	-2.417791	2.683273
H	2.174053	-1.971210	0.980086
H	3.050995	-3.380935	1.631364
C	0.871102	-4.895403	2.054804
H	0.009378	-5.452441	1.686484
H	0.727092	-4.691716	3.119803
H	-3.465065	4.790143	-0.179386
O	-0.138187	2.318832	0.795790
C	-1.227498	2.850508	0.952974
H	-1.630319	3.053018	1.960473
N	-2.049482	3.258306	-0.016447
C	-1.716279	3.059412	-1.405229
H	-2.403477	2.338923	-1.855898
H	-0.706622	2.662139	-1.475044
H	-1.785271	4.008301	-1.943950
C	-3.347349	3.805622	0.281002
H	-3.466656	3.909758	1.359497
H	-4.137633	3.149862	-0.096457
H	0.683742	-1.204094	-6.059608
O	0.525724	0.580126	-2.230592
C	0.459567	0.532590	-3.447347
H	0.731134	1.400351	-4.073481
N	0.069170	-0.518043	-4.178537
C	-0.326788	-1.759246	-3.557838
H	-1.375879	-1.975470	-3.783188
H	-0.191237	-1.694668	-2.480657
H	0.281061	-2.580917	-3.946438
C	0.022814	-0.453345	-5.617485
H	0.340895	0.533093	-5.955072
H	-0.993063	-0.634491	-5.980021
H	-3.848534	-3.899841	-0.210458
O	-2.172991	-0.003655	-0.253529
C	-2.917511	-0.909994	-0.588905
H	-3.321497	-0.979204	-1.614067
N	-3.343269	-1.908139	0.194229
C	-2.929189	-1.998391	1.573811
H	-3.753409	-1.731114	2.242938
H	-2.083450	-1.334677	1.745230
H	-2.628722	-3.024698	1.799178
C	-4.274454	-2.895337	-0.288175
H	-4.513453	-2.699142	-1.333480
H	-5.202291	-2.871163	0.290673
H	1.122417	1.795792	5.828815
O	-0.034389	-0.436404	2.417143
C	-0.189594	0.257586	3.411332
H	-1.099853	0.178451	4.031118
N	0.669536	1.163458	3.885054
C	1.925238	1.430074	3.224619
H	1.938236	2.454188	2.843927
H	2.049538	0.748769	2.387419
H	2.749128	1.302845	3.932239
C	0.363453	1.944739	5.055896
H	-0.605264	1.647864	5.458325
H	0.330118	3.010271	4.810230

DMSO SOLVENT

DMSO

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Charge of molecule: 0
Multiplicity: 1
E(HF/CC-PVTZ) = -551.64953467
```

E(DLPNO-CCSD(T)/CC-PVTZ) = -552.496963206
T1 (CC-PVTZ)= 0.013773201
T2 (CC-PVTZ)= 0.052039
E(HF/CC-PVQZ) = -551.67098625
E(DLPNO-CCSD(T)/CC-PVQZ) = -552.572955653
E(HF/DZ-CORE) = -551.57406065
E(DLPNO-CCSD(T)/DZ-CORE) = -552.505884804
E(HF/DZ-CORE (FC)) = -551.57406065
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -552.269214349
E(HF/TZ-CORE) = -551.66120218
E(DLPNO-CCSD(T)/TZ-CORE) = -552.937830219
E(HF/TZ-CORE (FC)) = -551.66120218
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -552.521068759
E(HF/TZ-IT) = -551.64953467
E(DLPNO-CCSD(T)/TZ-IT) = -552.498450142
E(IT_EFFECT) = -0.00148693627898
T1 (CC-PVQZ)= 0.013429972
T2 (CC-PVQZ)= 0.055156
E(HF/TZ-DKH) = -552.81134409
E(DLPNO-CCSDT/TZ-DKH) = -553.659296275
E(HF/CBS) = -551.683367318
E(DLPNO-CCSD(T)/CBS) = -552.616815716
E(DLPNO_TPNO/CC-PVTZ)) = -552.497219612
E(CV correction (DZ)) = -0.23667045532
E(CV correction (TZ)) = -0.416761459949
E(CV correction (CBS)) = -0.480138080384
E(TPNO_EFFECT) = -0.000256406190033
E(DKH correction) = -1.162333069
E(HF/TZ-SMD) = -551.66321718
E(DLPNO-CCSDT/TZ-SMD) = -552.508305709332
dG(solv_DLPNO_SMD) = -0.01108610
E(HF/TZ-PCM) = -551.66676293
E(DLPNO-CCSDT/TZ-PCM) = -552.51065307087
dG(solv_DLPNO_PCM) = -0.01343346
E(PBE0/TZ-GAS) = -552.969340432
E(PBE0/TZ-SMD) = -552.981204579
dG(solv_PBE0_SMD) = -0.011864147178
E(B3LYP/6-31G(d)-GAS) = -553.022377508482
E(B3LYP/6-31G(d)-SMD) = -553.032899269649
dG(solv_B3LYP_6-31G(d)_SMD) = -0.01052176
dGcorr (HO): 0.0499525500
dGcorr(HO(100)): 0.0499525500
dGcorr(qRRHO): 0.0513421500

C	-0.664765	0.001314	-5.128564
S	-1.479307	0.664759	-3.668508
O	-2.721148	-0.120117	-3.478882
C	-0.284258	0.043329	-2.476271
H	-1.305401	0.235067	-5.978538
H	0.309877	0.474834	-5.258589
H	-0.567645	-1.080542	-5.023082
H	0.685651	0.515626	-2.641546
H	-0.659974	0.307548	-1.488064
H	-0.216469	-1.041819	-2.570127

$Na^+(DMSO)_4$

Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -2368.46028224
E(DLPNO-CCSD(T)/CC-PVTZ) = -2372.1224503
T1 (CC-PVTZ)= 0.012256248
T2 (CC-PVTZ)= 0.053270
E(HF/CC-PVQZ) = -2368.53679505
E(DLPNO-CCSD(T)/CC-PVQZ) = -2372.45390658
E(HF/DZ-CORE) = -2368.18894144
E(DLPNO-CCSD(T)/DZ-CORE) = -2372.03935111
E(HF/DZ-CORE (FC)) = -2368.18894144
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -2371.0919964
E(HF/TZ-CORE) = -2368.50295223
E(DLPNO-CCSD(T)/TZ-CORE) = -2373.88056298
E(HF/TZ-CORE (FC)) = -2368.50295223
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -2372.21335803
E(HF/TZ-IT) = -2368.46028224
E(DLPNO-CCSD(T)/TZ-IT) = -2372.12829596
E(IT_EFFECT) = -0.00584565275312
T1 (CC-PVQZ)= 0.012087668
T2 (CC-PVQZ)= 0.055508
E(HF/TZ-DKH) = -2373.31637751
E(DLPNO-CCSDT/TZ-DKH) = -2376.98088789
E(HF/CBS) = -2368.58095545
E(DLPNO-CCSD(T)/CBS) = -2372.64521103
E(DLPNO_TPNO/CC-PVTZ)) = -2372.12299362
E(CV correction (DZ)) = -0.947354712922
E(CV correction (TZ)) = -1.66720494987
E(CV correction (CBS)) = -1.92053062447
E(TPNO_EFFECT) = -0.000543321470104
E(DKH correction) = -4.85843758488
E(HF/TZ-SMD) = -2368.52718069
E(DLPNO-CCSDT/TZ-SMD) = -2372.18801045395
dG(solv_DLPNO_SMD) = -0.06501683
E(HF/TZ-PCM) = -2368.53119451
E(DLPNO-CCSDT/TZ-PCM) = -2372.19063735393
dG(solv_DLPNO_PCM) = -0.06764373
E(PBE0/TZ-GAS) = -2374.07806691
E(PBE0/TZ-SMD) = -2374.14379933
dG(solv_PBE0_SMD) = -0.0657324223644
E(B3LYP/6-31G(d)-GAS) = -2374.3407408588
E(B3LYP/6-31G(d)-SMD) = -2374.40479846099
dG(solv_B3LYP_6-31G(d)_SMD) = -0.06405760
dGcorr (HO): 0.2504807400
dGcorr(HO(100)): 0.2631270000
dGcorr(qRRHO): 0.2664309300

Na	-0.499312	-0.393504	0.106843
C	1.308511	-1.844948	3.367314
S	0.757289	-2.861292	2.004326
O	-0.451964	-2.180130	1.435841
C	0.128159	-4.239803	2.949910
H	1.667253	-0.915373	2.924785
H	2.122633	-2.350889	3.888539
H	0.469467	-1.658214	4.039334
H	0.952950	-4.719062	3.479205
H	-0.310776	-4.940205	2.240076
H	-0.632275	-3.881369	3.644899
C	-1.569439	-1.111893	-4.435491
S	-1.123594	0.153799	-3.257054
O	-0.398089	-0.559123	-2.148531
C	-2.758983	0.514569	-2.635925
H	-0.644669	-1.482417	-4.876564
H	-2.195617	-0.670550	-5.212364
H	-2.092181	-1.917489	-3.918281
H	-3.340397	0.995399	-3.424070
H	-2.625605	1.195877	-1.794161
H	-3.238558	-0.409648	-2.308797
C	-2.015837	4.074967	1.114358
S	-0.703959	2.968163	0.618850
O	-1.385128	1.692788	0.207715
C	-0.004085	2.663054	2.234251
H	-2.588717	4.317032	0.219710
H	-1.578751	4.985563	1.526694
H	-2.651154	3.575740	1.847066
H	0.411931	3.593111	2.624692
H	0.789393	1.928512	2.089891
H	-0.780052	2.274046	2.895589
C	2.832173	-1.253885	-1.203652

S	2.884057	0.245909	-0.231041
O	1.666285	0.211650	0.654468
C	2.500758	1.393843	-1.547797
H	2.942993	-2.086539	-0.508827
H	3.670073	-1.248035	-1.902679
H	1.877585	-1.310742	-1.730745
H	3.316457	1.389544	-2.272341
H	2.416388	2.383260	-1.098914
H	1.558547	1.094939	-2.009386

$Na^+(DMSO)_5$

Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -2920.1286218
E(DLPNO-CCSD(T)/CC-PVTZ) = -2924.65673531
T1 (CC-PVTZ)= 0.012368277
T2 (CC-PVTZ)= 0.053583
E(HF/CC-PVQZ) = -2920.22300951
E(DLPNO-CCSD(T)/CC-PVQZ) = -2925.0604164
E(HF/DZ-CORE) = -2919.79133697
E(DLPNO-CCSD(T)/DZ-CORE) = -2924.59020996
E(HF/DZ-CORE (FC)) = -2919.79133697
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -2923.40614086
E(HF/TZ-CORE) = -2920.18192201
E(DLPNO-CCSD(T)/TZ-CORE) = -2926.85395803
E(HF/TZ-CORE (FC)) = -2920.18192201
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -2924.77008725
E(HF/TZ-IT) = -2920.1286218
E(DLPNO-CCSD(T)/TZ-IT) = -2924.66406967
E(IT_EFFECT) = -0.00733436097107
T1 (CC-PVQZ)= 0.012211887
T2 (CC-PVQZ)= 0.055665
E(HF/TZ-DKH) = -2926.14654697
E(DLPNO-CCSDT/TZ-DKH) = -2930.67754825
E(HF/CBS) = -2920.27748665
E(DLPNO-CCSD(T)/CBS) = -2925.29340638
E(DLPNO_TPNO/CC-PVTZ)) = -2924.65729159
E(CV correction (DZ)) = -1.18406910719
E(CV correction (TZ)) = -2.08387078639
E(CV correction (CBS)) = -2.40052396742
E(TPNO_EFFECT) = -0.000556281514037
E(DKH correction) = -6.02081294207
E(HF/TZ-SMD) = -2920.19172989
E(DLPNO-CCSDT/TZ-SMD) = -2924.71886413949
dG(solv_DLPNO_SMD) = -0.06157255
E(HF/TZ-PCM) = -2920.19739317
E(DLPNO-CCSDT/TZ-PCM) = -2924.72317607156
dG(solv_DLPNO_PCM) = -0.06588448
E(PBE0/TZ-GAS) = -2927.08742331
E(PBE0/TZ-SMD) = -2927.15024128
dG(solv_PBE0_SMD) = -0.0628179677169
E(B3LYP/6-31G(d)-GAS) = -2927.3921544681
E(B3LYP/6-31G(d)-SMD) = -2927.45270731374
dG(solv_B3LYP_6-31G(d)_SMD) = -0.06055285
dGcorr (HO): 0.3248597100
dGcorr(HO(100)): 0.3364442600
dGcorr(qRRHO): 0.3423910100

Na	-0.088332	-0.226155	0.200830
C	-2.298151	0.010360	-3.172182
S	-2.722682	-1.185841	-1.909476
O	-2.196724	-0.640357	-0.617071
C	-1.570507	-2.460892	-2.413631
H	-2.880769	0.907602	-2.963606
H	-2.580649	-0.385979	-4.148735
H	-1.227806	0.217819	-3.115294
H	-1.815533	-2.792037	-3.423758
H	-1.688104	-3.292082	-1.719435
H	-0.558515	-2.057518	-2.357923
C	-0.392045	3.342655	-1.550474
S	0.772713	3.074967	-0.223225
O	0.151144	2.060138	0.691825
C	0.579700	4.649003	0.602126
H	-0.404060	2.417382	-2.124940
H	-0.043085	4.167308	-2.173786
H	-1.375265	3.557314	-1.129227
H	0.927800	5.445353	-0.057292
H	1.198678	4.620260	1.498464
H	-0.468016	4.793091	0.869527
C	-0.779463	1.489474	3.939697
S	-1.689764	0.104247	3.266901
O	-0.708582	-0.646980	2.408929
C	-2.733957	1.029127	2.149282
H	-0.052187	1.087327	4.644424
H	-1.471240	2.149911	4.464914
H	-0.280952	2.001463	3.114768
H	-3.462954	1.589220	2.737015
H	-3.236036	0.302124	1.511308
H	-2.110624	1.689867	1.544561
C	3.320563	0.197324	-1.061809
S	2.236324	0.165289	-2.483723
O	0.835195	0.302782	-1.948941
C	2.442306	-1.563347	-2.892090
H	3.243600	1.193669	-0.626866
H	4.344277	0.022144	-1.396029
H	2.994855	-0.569238	-0.356585
H	3.483243	-1.740659	-3.166752
H	1.803112	-1.770173	-3.750328
H	2.148447	-2.157271	-2.024286
C	1.865432	-2.651977	2.681007
S	1.390376	-3.313337	1.089559
O	1.274357	-2.131671	0.161400
C	-0.281448	-3.779953	1.517930
H	2.873347	-2.252093	2.571761
H	1.873794	-3.463577	3.410282
H	1.156216	-1.870175	2.958812
H	-0.242359	-4.562863	2.276967
H	-0.744525	-4.176258	0.614851
H	-0.811149	-2.896786	1.880324

$Na^+(DMSO)_6$

Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -3471.78613217
E(DLPNO-CCSD(T)/CC-PVTZ) = -3477.18197186
T1 (CC-PVTZ)= 0.012528836
T2 (CC-PVTZ)= 0.053447
E(HF/CC-PVQZ) = -3471.89911097
E(DLPNO-CCSD(T)/CC-PVQZ) = -3477.658652
E(HF/DZ-CORE) = -3471.38218122
E(DLPNO-CCSD(T)/DZ-CORE) = -3477.13099022
E(HF/DZ-CORE (FC)) = -3471.38218122
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -3475.71008639
E(HF/TZ-CORE) = -3471.8509015
E(DLPNO-CCSD(T)/TZ-CORE) = -3479.81876759
E(HF/TZ-CORE (FC)) = -3471.8509015
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -3477.31825745
E(HF/TZ-IT) = -3471.78613217
E(DLPNO-CCSD(T)/TZ-IT) = -3477.1908363
E(IT_EFFECT) = -0.00886443064701
T1 (CC-PVQZ)= 0.012364511
T2 (CC-PVQZ)= 0.055241

```
E(HF/TZ-DKH) = -3478.96584671
E(DLPNO-CCSDT/TZ-DKH) = -3484.36511775
E(HF/CBS) = -3471.96431821
E(DLPNO-CCSD(T)/CBS) = -3477.93377435
E(DLPNO_TPNO/CC-PVTZ)) = -3477.18200917
E(CV correction (DZ)) = -1.42090382268
E(CV correction (TZ)) = -2.50051013648
E(CV correction (CBS)) = -2.8804391602
E(TPNO_EFFECT) = -3.73010002477e-05
E(DKH correction) = -7.18314588513
E(HF/TZ-SMD) = -3471.84738411
E(DLPNO-CCSDT/TZ-SMD) = -3477.24181363021
dG(solv_DLPNO_SMD) = -0.05980446
E(HF/TZ-PCM) = -3471.85671482
E(DLPNO-CCSDT/TZ-PCM) = -3477.24888144869
dG(solv_DLPNO_PCM) = -0.06687228
E(PBE0/TZ-GAS) = -3480.00933481
E(PBE0/TZ-SMD) = -3480.07054082
dG(solv_PBE0_SMD) = -0.0612060109552
E(B3LYP/6-31G(d)-GAS) = -3480.4297679104
E(B3LYP/6-31G(d)-SMD) = -3480.4880295211
dG(solv_B3LYP_6-31G(d)_SMD) = -0.05826161
dGcorr (HO): 0.3956657000
dGcorr(HO(100)): 0.4080961200
dGcorr(qRRHO): 0.4161882100
```

Na	0.038566	-0.026483	0.051269
C	-1.010909	-3.753058	3.158324
S	-1.201826	-2.095561	2.508701
O	-0.432488	-2.067736	1.227576
C	-2.928972	-2.218916	2.056243
H	0.032136	-3.866730	3.452463
H	-1.652613	-3.876191	4.032065
H	-1.263192	-4.476499	2.381665
H	-3.537190	-2.300008	2.958417
H	-3.161029	-1.299472	1.518542
H	-3.072390	-3.085794	1.409017
C	2.541259	-0.955475	2.802524
S	3.356863	-0.414413	1.304514
O	2.366845	-0.590907	0.191217
C	3.379245	1.336972	1.671022
H	2.353959	-2.022179	2.682882
H	3.214189	-0.790128	3.645598
H	1.605615	-0.405495	2.917668
H	3.991573	1.509665	2.557338
H	3.831408	1.832533	0.812109
H	2.349786	1.665624	1.822893
C	-2.334573	1.572244	3.113531
S	-0.714605	2.231348	2.735530
O	0.074588	1.094533	2.155045
C	-1.208259	3.263231	1.361509
H	-2.200990	0.834249	3.904046
H	-2.972756	2.382260	3.469969
H	-2.738378	1.114409	2.208776
H	-1.826976	4.078081	1.740828
H	-0.297033	3.653278	0.911238
H	-1.743354	2.647633	0.638298
C	-3.274412	-1.264154	-1.888322
S	-3.295795	0.400555	-1.232234
O	-2.376913	0.392494	-0.041952
C	-2.389287	1.174627	-2.564515
H	-3.767767	-1.907298	-1.160511
H	-3.830680	-1.281861	-2.826843
H	-2.233844	-1.558269	-2.035340
H	-3.018540	1.181559	-3.456103
H	-2.173323	2.195282	-2.250781
H	-1.464708	0.620160	-2.727183
C	2.302724	3.814872	-1.978055
S	1.796638	2.097745	-1.920596
O	0.600750	2.056259	-1.023470
C	1.178455	1.985670	-3.597266
H	2.671447	4.074670	-0.985904
H	3.104136	3.933167	-2.708926
H	1.444384	4.437775	-2.233963
H	2.008976	2.095572	-4.296477
H	0.735359	0.994394	-3.689197
H	0.425884	2.757912	-3.763204
C	1.124572	-3.261373	-1.290905
S	0.853906	-2.191856	-2.695250
O	0.099357	-0.991567	-2.186158
C	2.548229	-1.658086	-2.906980
H	0.145333	-3.577066	-0.934311
H	1.702397	-4.125188	-1.623927
H	1.639295	-2.699755	-0.510881
H	3.165649	-2.529130	-3.131983
H	2.571991	-0.972384	-3.753602
H	2.867286	-1.165740	-1.985978

ETHANOL SOLVENT

EtOH

```
Charge of molecule: 0
Multiplicity: 1
E(HF/CC-PVTZ) = -154.14235752
E(DLPNO-CCSD(T)/CC-PVTZ) = -154.794686635
T1 (CC-PVTZ)= 0.008465460
T2 (CC-PVTZ)= 0.041312
E(HF/CC-PVQZ) = -154.1541008
E(DLPNO-CCSD(T)/CC-PVQZ) = -154.844335504
E(HF/DZ-CORE) = -154.09343087
E(DLPNO-CCSD(T)/DZ-CORE) = -154.726760427
E(HF/DZ-CORE (FC)) = -154.09343087
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -
154.635193632
E(HF/TZ-CORE) = -154.14314887
E(DLPNO-CCSD(T)/TZ-CORE) = -154.953279129
E(HF/TZ-CORE (FC)) = -154.14314887
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -
154.803893885
E(HF/TZ-IT) = -154.14235752
E(DLPNO-CCSD(T)/TZ-IT) = -154.795399364
E(IT_EFFECT) = -0.000712729097984
T1 (CC-PVQZ)= 0.008806367
T2 (CC-PVQZ)= 0.047317
E(HF/TZ-DKH) = -154.22325249
E(DLPNO-CCSDT/TZ-DKH) = -154.875858317
E(HF/CBS) = -154.160878592
E(DLPNO-CCSD(T)/CBS) = -154.872991016
E(DLPNO_TPNO/CC-PVTZ)) = -154.794742416
E(CV correction (DZ)) = -0.091566795206
E(CV correction (TZ)) = -0.149385243774
E(CV correction (CBS)) = -0.169732389244
E(TPNO_EFFECT) = -5.57807929908e-05
E(DKH correction) = -0.081171681536
E(HF/TZ-SMD) = -154.15259028
E(DLPNO-CCSDT/TZ-SMD) = -154.80385032491
dG(solv_DLPNO_SMD) = -0.00910791
E(HF/TZ-PCM) = -154.14989945
E(DLPNO-CCSDT/TZ-PCM) = -154.801488653213
dG(solv_DLPNO_PCM) = -0.00674624
E(PBE0/TZ-GAS) = -154.921151893
E(PBE0/TZ-SMD) = -154.930913646
dG(solv_PBE0_SMD) = -0.009761753014
E(B3LYP/6-31G(d)-GAS) = -154.935759696485
E(B3LYP/6-31G(d)-SMD) = -154.945075315742
dG(solv_B3LYP_6-31G(d)_SMD) = -0.00931562
dGcorr (HO): 0.0533911600
```

```
dGcorr(HO(100)): 0.0533911600
dGcorr(qRRHO): 0.0547719800

 C     0.013978    -0.552523    -0.032101
 H     0.067744    -1.236734     0.817789
 H     0.041260    -1.166979    -0.942975
 C    -1.269666     0.247026     0.019143
 H    -2.140088    -0.413792    -0.006190
 H    -1.314004     0.844422     0.932032
 H    -1.344788     0.925064    -0.836753
 O     1.168917     0.256348     0.061349
 H     1.154139     0.885210    -0.664514
```

$Na^+(EtOH)_4$

```
Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -778.37920155
E(DLPNO-CCSD(T)/CC-PVTZ) = -781.261630052
T1 (CC-PVTZ)= 0.008277164
T2 (CC-PVTZ)= 0.041773
E(HF/CC-PVQZ) = -778.42230651
E(DLPNO-CCSD(T)/CC-PVQZ) = -781.492717173
E(HF/DZ-CORE) = -778.19858608
E(DLPNO-CCSD(T)/DZ-CORE) = -780.859327397
E(HF/DZ-CORE (FC)) = -778.19858608
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -
780.492896411
E(HF/TZ-CORE) = -778.38223047
E(DLPNO-CCSD(T)/TZ-CORE) = -781.895493869
E(HF/TZ-CORE (FC)) = -778.38223047
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -
781.297985374
E(HF/TZ-IT) = -778.37920155
E(DLPNO-CCSD(T)/TZ-IT) = -781.264571484
E(IT_EFFECT) = -0.00294143192104
T1 (CC-PVQZ)= 0.008359986
T2 (CC-PVQZ)= 0.046376
E(HF/TZ-DKH) = -778.91157157
E(DLPNO-CCSDT/TZ-DKH) = -781.795389381
E(HF/CBS) = -778.447185118
E(DLPNO-CCSD(T)/CBS) = -781.626092215
E(DLPNO_TPNO/CC-PVTZ)) = -781.262157106
E(CV correction (DZ)) = -0.366430985707
E(CV correction (TZ)) = -0.597508495238
E(CV correction (CBS)) = -0.678828001689
E(TPNO_EFFECT) = -0.000527053489009
E(DKH correction) = -0.533759328509
E(HF/TZ-SMD) = -778.46099234
E(DLPNO-CCSDT/TZ-SMD) = -781.343675227656
dG(solv_DLPNO_SMD) = -0.08151812
E(HF/TZ-PCM) = -778.44964628
E(DLPNO-CCSDT/TZ-PCM) = -781.332478806485
dG(solv_DLPNO_PCM) = -0.07032170
E(PBE0/TZ-GAS) = -781.801747172
E(PBE0/TZ-SMD) = -781.884250649
dG(solv_PBE0_SMD) = -0.0825034761081
E(B3LYP/6-31G(d)-GAS) = -781.9462057199
E(B3LYP/6-31G(d)-SMD) = -782.028481120783
dG(solv_B3LYP_6-31G(d)_SMD) = -0.08227540
dGcorr (HO): 0.2624280000
dGcorr(HO(100)): 0.2724938100
dGcorr(qRRHO): 0.2770131600

Na    0.001510    -0.009850    -0.004539
 C    1.299795     2.354028     1.962547
 H    1.868448     2.122689     2.868624
 H    0.873901     3.356180     2.072316
 C    2.184864     2.283528     0.747848
 H    3.001917     3.000477     0.839420
 H    2.622250     1.287741     0.639540
 H    1.625274     2.525961    -0.159208
 O    0.239273     1.399849     1.809079
 H   -0.328751     1.448806     2.581914
 C   -2.409454    -2.263050    -0.481948
 H   -3.431558    -1.987398    -0.759791
 H   -2.441204    -3.236189     0.017748
 C   -1.525646    -2.319445    -1.698347
 H   -1.905909    -3.061015    -2.402215
 H   -1.500302    -1.353434    -2.208909
 H   -0.505701    -2.605108    -1.428144
 O   -1.879412    -1.281244     0.420087
 H   -2.439397    -1.249246     1.199608
 C    2.371687    -2.240930     0.727684
 H    3.391810    -1.954993     1.002333
 H    2.399710    -3.253849     0.314287
 C    1.463198    -2.181843     1.925646
 H    1.818483    -2.866222     2.697281
 H    1.442738    -1.175967     2.352907
 H    0.444649    -2.475497     1.659273
 O    1.873986    -1.334233    -0.266812
 H    2.451401    -1.375696    -1.033064
 C   -1.257873     2.154379    -2.202535
 H   -1.846407     1.861033    -3.077356
 H   -0.798176     3.125843    -2.409315
 C   -2.129001     2.229594    -0.977950
 H   -2.921335     2.964201    -1.128178
 H   -2.600138     1.264957    -0.772490
 H   -1.549602     2.534928    -0.102916
 O   -0.230146     1.180161    -1.971224
 H    0.325118     1.130852    -2.753201
```

$Na^+(EtOH)_5$

```
Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -932.53913324
E(DLPNO-CCSD(T)/CC-PVTZ) = -936.083219824
T1 (CC-PVTZ)= 0.008382078
T2 (CC-PVTZ)= 0.046570
E(HF/CC-PVQZ) = -932.5927117
E(DLPNO-CCSD(T)/CC-PVQZ) = -936.36255258
E(HF/DZ-CORE) = -932.31414187
E(DLPNO-CCSD(T)/DZ-CORE) = -935.615806782
E(HF/DZ-CORE (FC)) = -932.31414187
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -
935.157812154
E(HF/TZ-CORE) = -932.54290633
E(DLPNO-CCSD(T)/TZ-CORE) = -936.875612574
E(HF/TZ-CORE (FC)) = -932.54290633
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -
936.128770212
E(HF/TZ-IT) = -932.53913324
E(DLPNO-CCSD(T)/TZ-IT) = -936.086914967
E(IT_EFFECT) = -0.003695142776
T1 (CC-PVQZ)= 0.008464244
T2 (CC-PVQZ)= 0.049253
E(HF/TZ-DKH) = -933.15236114
E(DLPNO-CCSDT/TZ-DKH) = -936.698117035
E(HF/CBS) = -932.623635229
E(DLPNO-CCSD(T)/CBS) = -936.52377324
E(DLPNO_TPNO/CC-PVTZ)) = -936.083996644
E(CV correction (DZ)) = -0.457994627857
E(CV correction (TZ)) = -0.746842361192
E(CV correction (CBS)) = -0.848492042123
E(TPNO_EFFECT) = -0.000776820069063
E(DKH correction) = -0.614897211257
E(HF/TZ-SMD) = -932.61798999
```

```
E(DLPNO-CCSDT/TZ-SMD) = -936.162471691374
dG(solv_DLPNO_SMD) = -0.07847505
E(HF/TZ-PCM) = -932.60578957
E(DLPNO-CCSDT/TZ-PCM) = -936.150440006437
dG(solv_DLPNO_PCM) = -0.06644336
E(PBE0/TZ-GAS) = -936.781900643
E(PBE0/TZ-SMD) = -936.861334501
dG(solv_PBE0_SMD) = -0.0794338582031
E(B3LYP/6-31G(d)-GAS) = -936.9102755482
E(B3LYP/6-31G(d)-SMD) = -936.989242507966
dG(solv_B3LYP_6-31G(d)_SMD) = -0.07896696
dGcorr (HO): 0.3344632600
dGcorr(HO(100)): 0.3479819700
dGcorr(qRRHO): 0.3529774500

Na    -0.084176     0.479079     0.820419
 C     3.148705    -0.481438     0.239826
 H     3.723673    -0.198416    -0.649125
 H     3.483850    -1.476822     0.553010
 C     3.370788     0.517604     1.345021
 H     4.426955     0.561306     1.614609
 H     3.061427     1.516289     1.027038
 H     2.806837     0.241045     2.239917
 O     1.760936    -0.513460    -0.070436
 H     1.593799    -1.114266    -0.814084
 C    -2.663311    -1.249289    -0.645943
 H    -2.707298    -2.312225    -0.381378
 H    -3.069927    -1.138912    -1.657283
 C    -3.464842    -0.433140     0.333395
 H    -4.502736    -0.769018     0.347331
 H    -3.063199    -0.533024     1.345018
 H    -3.457245     0.623442     0.056835
 O    -1.311645    -0.801591    -0.618383
 H    -0.778005    -1.316956    -1.244144
 C     0.928865    -1.473632    -3.532065
 H     0.243907    -1.953753    -4.236727
 H     1.953871    -1.705113    -3.836553
 C     0.702779     0.013411    -3.493789
 H     0.887829     0.438707    -4.481289
 H    -0.325834     0.246483    -3.211147
 H     1.378129     0.495389    -2.783616
 O     0.698578    -2.006674    -2.214006
 H     0.801352    -2.962727    -2.241196
 C    -0.646939    -1.183507     3.665670
 H    -1.665434    -1.415272     3.993713
 H    -0.004116    -1.143438     4.550652
 C    -0.152458    -2.225058     2.698232
 H    -0.149215    -3.205649     3.176477
 H    -0.796888    -2.279368     1.817446
 H     0.866287    -2.005169     2.370288
 O    -0.634652     0.089507     3.008338
 H    -0.954599     0.757830     3.619224
 C    -0.229904     3.685383    -0.153859
 H     0.613081     3.922939    -0.811238
 H    -0.571267     4.613806     0.313728
 C    -1.348323     3.047055    -0.931971
 H    -1.685132     3.719521    -1.722363
 H    -1.024954     2.115116    -1.403416
 H    -2.201530     2.835769    -0.283766
 O     0.198277     2.769268     0.861316
 H     0.843702     3.208968     1.420270
```

$Na^+(EtOH)_6$

```
Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -1086.68655504
E(DLPNO-CCSD(T)/CC-PVTZ) = -1090.89456292
T1 (CC-PVTZ)= 0.008445621
T2 (CC-PVTZ)= 0.042553
E(HF/CC-PVQZ) = -1086.75015637
E(DLPNO-CCSD(T)/CC-PVQZ) = -1091.22127549
E(HF/DZ-CORE) = -1086.41662538
E(DLPNO-CCSD(T)/DZ-CORE) = -1090.36413385
E(HF/DZ-CORE (FC)) = -1086.41662538
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -
1089.81455522
E(HF/TZ-CORE) = -1086.69113172
E(DLPNO-CCSD(T)/TZ-CORE) = -1091.84478338
E(HF/TZ-CORE (FC)) = -1086.69113172
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -
1090.94868313
E(HF/TZ-IT) = -1086.68655504
E(DLPNO-CCSD(T)/TZ-IT) = -1090.89899008
E(IT_EFFECT) = -0.00442716419707
T1 (CC-PVQZ)= 0.008553525
T2 (CC-PVQZ)= 0.046751
E(HF/TZ-DKH) = -1087.38071754
E(DLPNO-CCSDT/TZ-DKH) = -1091.59067495
E(HF/CBS) = -1086.78686473
E(DLPNO-CCSD(T)/CBS) = -1091.40984205
E(DLPNO_TPNO/CC-PVTZ)) = -1090.89479394
E(CV correction (DZ)) = -0.549578626253
E(CV correction (TZ)) = -0.896100249138
E(CV correction (CBS)) = -1.01804620314
E(TPNO_EFFECT) = -0.000231018010936
E(DKH correction) = -0.69611202695
E(HF/TZ-SMD) = -1086.77470153
E(DLPNO-CCSDT/TZ-SMD) = -1090.98135908676
dG(solv_DLPNO_SMD) = -0.08656515
E(HF/TZ-PCM) = -1086.75807159
E(DLPNO-CCSDT/TZ-PCM) = -1090.96551735574
dG(solv_DLPNO_PCM) = -0.07072342
E(PBE0/TZ-GAS) = -1091.7193425
E(PBE0/TZ-SMD) = -1091.80723773
dG(solv_PBE0_SMD) = -0.0878952302189
E(B3LYP/6-31G(d)-GAS) = -1091.8540371550
E(B3LYP/6-31G(d)-SMD) = -1091.9421799528
dG(solv_B3LYP_6-31G(d)_SMD) = -0.08814280
dGcorr (HO): 0.4053226400
dGcorr(HO(100)): 0.4189410500
dGcorr(qRRHO): 0.4263691700

Na    -0.000602     0.006146     0.002184
 C    -1.285019     0.897325     3.011274
 H    -0.273136     0.532702     3.198384
 H    -1.940151     0.432894     3.756324
 C    -1.348959     2.402731     3.105840
 H    -1.047273     2.735439     4.101533
 H    -0.689165     2.867418     2.369888
 H    -2.364793     2.768546     2.933124
 O    -1.615083     0.416039     1.710177
 H    -2.527859     0.645992     1.518308
 C    -1.810250    -1.936110    -2.101134
 H    -1.425742    -1.101629    -2.690627
 H    -2.872492    -2.044402    -2.346120
 C    -1.058476    -3.209905    -2.403032
 H    -1.155362    -3.468570    -3.459827
 H     0.002531    -3.100294    -2.168402
 H    -1.451833    -4.049859    -1.823916
 O    -1.666698    -1.524499    -0.743413
 H    -2.049945    -2.197351    -0.174868
 C     2.919884    -0.838554    -1.496615
 H     3.178156    -0.438799    -0.514067
 H     3.595078    -0.374015    -2.223525
 C     3.053135    -2.342018    -1.526566
 H     4.079274    -2.638881    -1.298580
 H     2.386968    -2.806346    -0.796318
 H     2.809550    -2.742062    -2.514672
 O     1.582637    -0.403099    -1.731769
```

H	1.319650	-0.677466	-2.614107
C	2.214125	2.572987	0.012504
H	2.145877	2.228257	-1.021115
H	3.277932	2.691475	0.245463
C	1.475505	3.875744	0.203249
H	1.896003	4.650735	-0.441444
H	0.416295	3.761401	-0.037132
H	1.555696	4.229909	1.234639
O	1.663706	1.513135	0.791791
H	1.759253	1.732616	1.722160
C	-2.329542	1.781290	-1.687218
H	-2.855973	0.943951	-1.225019
H	-2.685510	1.857840	-2.720349
C	-2.582470	3.066390	-0.936382
H	-3.649774	3.298475	-0.925532
H	-2.233133	2.988669	0.095456
H	-2.070020	3.909183	-1.408311
O	-0.954662	1.402983	-1.676145
H	-0.445635	2.077739	-2.132904
C	0.279710	-2.482097	2.272276
H	-0.769766	-2.181234	2.264212
H	0.583207	-2.572186	3.320972
C	0.478533	-3.788973	1.543106
H	-0.106001	-4.581973	2.014901
H	0.168712	-3.703135	0.499392
H	1.526710	-4.099650	1.564352
O	0.977344	-1.400741	1.658038
H	1.919855	-1.584160	1.689561

ACETONE SOLVENT

Me_2CO

```
Charge of molecule: 0
Multiplicity: 1
E(HF/CC-PVTZ) = -192.03427079
E(DLPNO-CCSD(T)/CC-PVTZ) = -192.834890182
T1 (CC-PVTZ)= 0.012691337
T2 (CC-PVTZ)= 0.056947
E(HF/CC-PVQZ) = -192.04809844
E(DLPNO-CCSD(T)/CC-PVQZ) = -192.894092834
E(HF/DZ-CORE) = -191.97903232
E(DLPNO-CCSD(T)/DZ-CORE) = -192.772301293
E(HF/DZ-CORE (FC)) = -191.97903232
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -
192.650567854
E(HF/TZ-CORE) = -192.03554911
E(DLPNO-CCSD(T)/TZ-CORE) = -193.044654992
E(HF/TZ-CORE (FC)) = -192.03554911
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -
192.846980859
E(HF/TZ-IT) = -192.03427079
E(DLPNO-CCSD(T)/TZ-IT) = -192.836219734
E(IT_EFFECT) = -0.00132955197901
T1 (CC-PVQZ)= 0.012474098
T2 (CC-PVQZ)= 0.056249
E(HF/TZ-DKH) = -192.12997411
E(DLPNO-CCSDT/TZ-DKH) = -192.930915296
E(HF/CBS) = -192.056079254
E(DLPNO-CCSD(T)/CBS) = -192.928262442
E(DLPNO_TPNO/CC-PVTZ)) = -192.835108149
E(CV correction (DZ)) = -0.12173343878
E(CV correction (TZ)) = -0.197674133401
E(CV correction (CBS)) = -0.224398758479
E(TPNO_EFFECT) = -0.000217967275006
E(DKH correction) = -0.096025114361
E(HF/TZ-SMD) = -192.04545441
E(DLPNO-CCSDT/TZ-SMD) = -192.844128695845
dG(solv_DLPNO_SMD) = -0.00902055
E(HF/TZ-PCM) = -192.04425281
E(DLPNO-CCSDT/TZ-PCM) = -192.842326373449
dG(solv_DLPNO_PCM) = -0.00721822
E(PBE0/TZ-GAS) = -193.003149728
E(PBE0/TZ-SMD) = -193.01333359
dG(solv_PBE0_SMD) = -0.010183861175
E(B3LYP/6-31G(d)-GAS) = -193.03402143502
E(B3LYP/6-31G(d)-SMD) = -193.042823913026
dG(solv_B3LYP_6-31G(d)_SMD) = -0.00880248
dGcorr (HO): 0.0534551100
dGcorr(HO(100)): 0.0551735700
dGcorr(qRRHO): 0.0560818600
```

C	-1.279672	0.000049	-0.153087
H	-1.318368	-0.877589	-0.804520
H	-1.318950	0.877925	-0.804160
H	-2.136551	-0.000357	0.517601
C	1.279673	-0.000011	-0.153076
H	1.318817	0.877591	-0.804523
H	2.136544	-0.000023	0.517622
H	1.318518	-0.877922	-0.804136
C	-0.000003	0.000380	0.641292
O	-0.000007	-0.000042	1.846987

$Na^+(Me_2CO)_4$

```
Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -929.96750599
E(DLPNO-CCSD(T)/CC-PVTZ) = -933.4299641
T1 (CC-PVTZ)= 0.012644031
T2 (CC-PVTZ)= 0.053286
E(HF/CC-PVQZ) = -930.02009724
E(DLPNO-CCSD(T)/CC-PVQZ) = -933.701972853
E(HF/DZ-CORE) = -929.75664318
E(DLPNO-CCSD(T)/DZ-CORE) = -933.039401645
E(HF/DZ-CORE (FC)) = -929.75664318
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -
932.552172849
E(HF/TZ-CORE) = -929.97219724
E(DLPNO-CCSD(T)/TZ-CORE) = -934.267923001
E(HF/TZ-CORE (FC)) = -929.97219724
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -
933.477148109
E(HF/TZ-IT) = -929.96750599
E(DLPNO-CCSD(T)/TZ-IT) = -933.435266568
E(IT_EFFECT) = -0.00530246709798
T1 (CC-PVQZ)= 0.012402907
T2 (CC-PVQZ)= 0.053195
E(HF/TZ-DKH) = -930.55908909
E(DLPNO-CCSDT/TZ-DKH) = -934.023120156
E(HF/CBS) = -930.050450988
E(DLPNO-CCSD(T)/CBS) = -933.858966366
E(DLPNO_TPNO/CC-PVTZ)) = -933.430717689
E(CV correction (DZ)) = -0.487228795982
E(CV correction (TZ)) = -0.790774892165
E(CV correction (CBS)) = -0.897597138851
E(TPNO_EFFECT) = -0.000753588216071
E(DKH correction) = -0.593156055365
E(HF/TZ-SMD) = -930.03883937
E(DLPNO-CCSDT/TZ-SMD) = -933.499691017851
dG(solv_DLPNO_SMD) = -0.06897333
E(HF/TZ-PCM) = -930.0291561
E(DLPNO-CCSDT/TZ-PCM) = -933.489817192488
dG(solv_DLPNO_PCM) = -0.05909950
E(PBE0/TZ-GAS) = -934.175612078
E(PBE0/TZ-SMD) = -934.245585601
```

```
dG(solv_PBE0_SMD) = -0.0699735230249
E(B3LYP/6-31G(d)-GAS) = -934.3535514748
E(B3LYP/6-31G(d)-SMD) = -934.422102083641
dG(solv_B3LYP_6-31G(d)_SMD) = -0.06855061
dGcorr (HO): 0.2598261000
dGcorr(HO(100)): 0.2777766500
dGcorr(qRRHO): 0.2797523900

Na     0.397917     0.204067    -0.067166
 C     0.158593    -4.326703    -0.993417
 H    -0.682424    -4.636836    -1.621893
 H     0.322986    -5.133837    -0.275918
 H     1.039830    -4.185326    -1.615335
 C    -1.244316    -3.141614     0.783537
 H    -0.817911    -3.667207     1.643991
 H    -1.567868    -2.148390     1.091642
 H    -2.099158    -3.735283     0.451966
 C    -0.205781    -3.058528    -0.291508
 O     0.322733    -2.001987    -0.583375
 C    -3.771411     1.413859     1.578969
 H    -4.715078     1.308058     1.038686
 H    -3.812629     2.382977     2.085905
 H    -3.667275     0.623343     2.319027
 C    -2.695109     2.320247    -0.554036
 H    -2.944035     3.335751    -0.236039
 H    -1.762436     2.318418    -1.116329
 H    -3.512661     1.992237    -1.203333
 C    -2.616279     1.408764     0.629953
 O    -1.651124     0.690537     0.819211
 C     1.031859     0.676954     3.761015
 H     1.089449     1.529938     4.441302
 H     1.167738    -0.218054     4.376107
 H     0.055721     0.641392     3.279630
 C     3.515470     0.986933     3.241374
 H     3.745665     0.335055     4.087275
 H     4.241773     0.847985     2.443703
 H     3.579603     2.014048     3.614464
 C     2.128346     0.739162     2.743283
 O     1.901599     0.594524     1.557030
 C     0.958022     2.123621    -4.239059
 H     0.282506     1.773459    -5.026206
 H     1.930419     2.278395    -4.712361
 H     0.580916     3.057672    -3.828404
 C     1.774986    -0.188460    -3.521153
 H     2.849877     0.021429    -3.520121
 H     1.563988    -0.971187    -2.793507
 H     1.524963    -0.524894    -4.529299
 C     1.047827     1.074261    -3.179499
 O     0.552709     1.245226    -2.080112
```

$Na^+(Me_2CO)_5$

```
Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -1122.01122001
E(DLPNO-CCSD(T)/CC-PVTZ) = -1126.28735171
T1 (CC-PVTZ)= 0.012692016
T2 (CC-PVTZ)= 0.054606
E(HF/CC-PVQZ) = -1122.0761004
E(DLPNO-CCSD(T)/CC-PVQZ) = -1126.61684616
E(HF/DZ-CORE) = -1121.74952943
E(DLPNO-CCSD(T)/DZ-CORE) = -1125.83750006
E(HF/DZ-CORE (FC)) = -1121.74952943
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -
1125.22855549
E(HF/TZ-CORE) = -1122.01710922
E(DLPNO-CCSD(T)/TZ-CORE) = -1127.33447275
E(HF/TZ-CORE (FC)) = -1122.01710922
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -
1126.34611167
E(HF/TZ-IT) = -1122.01122001
E(DLPNO-CCSD(T)/TZ-IT) = -1126.29401752
E(IT_EFFECT) = -0.00666581282189
T1 (CC-PVQZ)= 0.012455611
T2 (CC-PVQZ)= 0.054798
E(HF/TZ-DKH) = -1122.69849451
E(DLPNO-CCSDT/TZ-DKH) = -1126.97652326
E(HF/CBS) = -1122.11354699
E(DLPNO-CCSD(T)/CBS) = -1126.80701831
E(DLPNO_TPNO/CC-PVTZ)) = -1126.2881285
E(CV correction (DZ)) = -0.60894457131
E(CV correction (TZ)) = -0.988361079831
E(CV correction (CBS)) = -1.12188321825
E(TPNO_EFFECT) = -0.000776792740908
E(DKH correction) = -0.689171556315
E(HF/TZ-SMD) = -1122.0831813
E(DLPNO-CCSDT/TZ-SMD) = -1126.35727013822
dG(solv_DLPNO_SMD) = -0.06914164
E(HF/TZ-PCM) = -1122.07303043
E(DLPNO-CCSDT/TZ-PCM) = -1126.34644493652
dG(solv_DLPNO_PCM) = -0.05831644
E(PBE0/TZ-GAS) = -1127.20416149
E(PBE0/TZ-SMD) = -1127.27462359
dG(solv_PBE0_SMD) = -0.0704621036491
E(B3LYP/6-31G(d)-GAS) = -1127.4048626439
E(B3LYP/6-31G(d)-SMD) = -1127.47358476979
dG(solv_B3LYP_6-31G(d)_SMD) = -0.06872213
dGcorr (HO): 0.3334082200
dGcorr(HO(100)): 0.3535422000
dGcorr(qRRHO): 0.3570357300

Na    -0.057867     0.127832    -0.237769
 C    -1.970345     0.935840     2.965526
 H    -2.959965     1.272745     2.637818
 H    -1.934677     1.064434     4.048372
 H    -1.208294     1.543945     2.479963
 C    -2.400341    -1.527027     3.498303
 H    -1.824055    -1.535941     4.428856
 H    -2.374698    -2.516647     3.046717
 H    -3.423944    -1.259943     3.772663
 C    -1.818891    -0.501921     2.576551
 O    -1.255896    -0.826873     1.548592
 C    -3.154624    -2.592809    -2.429147
 H    -2.882664    -3.140108    -3.337418
 H    -3.775331    -3.267932    -1.835039
 H    -3.714836    -1.700574    -2.700496
 C    -1.155044    -3.354708    -1.033161
 H    -1.634604    -3.562226    -0.070980
 H    -0.123640    -3.061120    -0.848724
 H    -1.198570    -4.270826    -1.623958
 C    -1.905155    -2.235746    -1.688660
 O    -1.519491    -1.086260    -1.613115
 C    -0.031472     3.672229    -3.334724
 H     0.346770     3.372435    -4.317225
 H    -0.801623     4.425652    -3.514737
 H     0.783972     4.094814    -2.751380
 C    -1.896107     1.933601    -3.198835
 H    -2.704298     2.612387    -2.906356
 H    -2.096287     0.939291    -2.803883
 H    -1.881605     1.921351    -4.290849
 C    -0.609508     2.470314    -2.654236
 O    -0.054642     1.960900    -1.699981
 C     2.907268     2.213121     0.027266
 H     2.666955     2.852653    -0.827943
 H     3.901105     2.498479     0.376439
 H     2.896131     1.176977    -0.307370
 C     2.018847     3.669022     1.928738
 H     2.889845     3.546297     2.580009
 H     1.132049     3.830641     2.537872
```

H	2.218736	4.545051	1.306773
C	1.867004	2.446366	1.079429
O	0.932688	1.684274	1.231278
C	1.802367	-2.788149	1.557097
H	1.768849	-3.848735	1.288619
H	2.397439	-2.721711	2.471297
H	0.792131	-2.422761	1.733548
C	3.909840	-2.287411	0.198209
H	4.493443	-1.898933	1.038926
H	4.235206	-1.805137	-0.721099
H	4.106936	-3.361029	0.154871
C	2.458933	-2.021726	0.450098
O	1.841962	-1.214396	-0.216749

$Na^+(Me_2CO)_6$

Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -1314.05579899
E(DLPNO-CCSD(T)/CC-PVTZ) = -1319.14708101
T1 (CC-PVTZ)= 0.012693388
T2 (CC-PVTZ)= 0.054849
E(HF/CC-PVQZ) = -1314.13295238
E(DLPNO-CCSD(T)/CC-PVQZ) = -1319.53411622
E(HF/DZ-CORE) = -1313.74361135
E(DLPNO-CCSD(T)/DZ-CORE) = -1318.63842178
E(HF/DZ-CORE (FC)) = -1313.74361135
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -1317.9077041
E(HF/TZ-CORE) = -1314.06287658
E(DLPNO-CCSD(T)/TZ-CORE) = -1320.40323388
E(HF/TZ-CORE (FC)) = -1314.06287658
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -1319.21734237
E(HF/TZ-IT) = -1314.05579899
E(DLPNO-CCSD(T)/TZ-IT) = -1319.1550948
E(IT_EFFECT) = -0.00801378310598
T1 (CC-PVQZ)= 0.012470004
T2 (CC-PVQZ)= 0.054679
E(HF/TZ-DKH) = -1314.83877177
E(DLPNO-CCSDT/TZ-DKH) = -1319.93227642
E(HF/CBS) = -1314.1774825
E(DLPNO-CCSD(T)/CBS) = -1319.75749879
E(DLPNO_TPNO/CC-PVTZ)) = -1319.14783649
E(CV correction (DZ)) = -0.730717681855
E(CV correction (TZ)) = -1.18589150723
E(CV correction (CBS)) = -1.34607373744
E(TPNO_EFFECT) = -0.000755476316954
E(DKH correction) = -0.785195404221
E(HF/TZ-SMD) = -1314.12744748
E(DLPNO-CCSDT/TZ-SMD) = -1319.21685721726
dG(solv_DLPNO_SMD) = -0.06902073
E(HF/TZ-PCM) = -1314.11711436
E(DLPNO-CCSDT/TZ-PCM) = -1319.20527297237
dG(solv_DLPNO_PCM) = -0.05743648
E(PBE0/TZ-GAS) = -1320.17978714
E(PBE0/TZ-SMD) = -1320.25024845
dG(solv_PBE0_SMD) = -0.0704613064211
E(B3LYP/6-31G(d)-GAS) = -1320.4566347424
E(B3LYP/6-31G(d)-SMD) = -1320.52513229862
dG(solv_B3LYP_6-31G(d)_SMD) = -0.06849756
dGcorr (HO): 0.4131494500
dGcorr(HO(100)): 0.4312907600
dGcorr(qRRHO): 0.4381220500

Na	-0.000301	-0.000127	-0.000123
C	-0.240453	-1.302029	-4.546011
H	0.540380	-1.929468	-4.983058
H	-1.192199	-1.672718	-4.938959
H	-0.107076	-0.264732	-4.846707
C	-0.207333	-2.814699	-2.487084
H	-0.812242	-3.501861	-3.081646
H	-0.526863	-2.814130	-1.446445
H	0.826712	-3.171745	-2.540578
C	-0.245079	-1.428312	-3.053369
O	-0.266248	-0.446553	-2.339166
C	0.207254	2.814800	2.487333
H	-0.826768	3.171926	2.540823
H	0.812179	3.501819	3.082042
H	0.526835	2.814358	1.446707
C	0.239976	1.301606	4.545914
H	1.191708	1.672062	4.939112
H	0.106399	0.264260	4.846356
H	-0.540856	1.929045	4.982966
C	0.244811	1.428275	3.053315
O	0.265965	0.446753	2.338795
C	-2.741839	-3.470473	1.704547
H	-2.797697	-3.665371	2.778412
H	-3.762836	-3.557597	1.320160
H	-2.110064	-4.209755	1.216143
C	-2.872685	-0.972786	2.225604
H	-3.942808	-1.141688	2.359020
H	-2.685169	-0.012225	1.749161
H	-2.423077	-0.966239	3.224341
C	-2.239586	-2.083349	1.444800
O	-1.350071	-1.875888	0.644517
C	2.871469	0.972679	-2.226533
H	2.421402	0.967415	-3.225074
H	3.941648	1.140955	-2.360250
H	2.683440	0.011816	-1.750916
C	2.743212	3.469925	-1.702927
H	3.764454	3.555533	-1.318868
H	2.112397	4.209346	-1.213492
H	2.798819	3.665933	-2.776608
C	2.239496	2.083054	-1.444550
O	1.349713	1.875777	-0.644525
C	-1.686401	2.693426	-1.995240
H	-2.459072	3.016688	-2.695283
H	-0.977923	3.522673	-1.895650
H	-1.155728	1.821648	-2.373792
C	-3.342433	3.334687	-0.158564
H	-3.048325	4.378299	-0.296130
H	-3.578465	3.141215	0.885971
H	-4.239685	3.182945	-0.766351
C	-2.262029	2.415863	-0.640560
O	-1.864972	1.496775	0.046742
C	1.687583	-2.692323	1.995492
H	0.979442	-3.522012	1.897154
H	2.460937	-3.014669	2.695207
H	1.156809	-1.820470	2.373725
C	3.341991	-3.334790	0.157738
H	4.239847	-3.182567	0.764512
H	3.576966	-3.141995	-0.887162
H	3.048066	-4.378321	0.296286
C	2.262018	-2.415663	0.640127
O	1.864356	-1.497003	-0.047400

ACETONITRILE SOLVENT

MeCN

Charge of molecule: 0
Multiplicity: 1
E(HF/CC-PVTZ) = -131.97377588
E(DLPNO-CCSD(T)/CC-PVTZ) = -132.526373938
T1 (CC-PVTZ)= 0.012097424

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T2 (CC-PVTZ)= 0.060927
E(HF/CC-PVQZ) = -131.9826654
E(DLPNO-CCSD(T)/CC-PVQZ) = -132.56452327
E(HF/DZ-CORE) = -131.93977579
E(DLPNO-CCSD(T)/DZ-CORE) = -132.499275171
E(HF/DZ-CORE (FC)) = -131.93977579
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -
132.408182343
E(HF/TZ-CORE) = -131.97525347
E(DLPNO-CCSD(T)/TZ-CORE) = -132.682399237
E(HF/TZ-CORE (FC)) = -131.97525347
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -
132.53516857
E(HF/TZ-IT) = -131.97377588
E(DLPNO-CCSD(T)/TZ-IT) = -132.527527342
E(IT_EFFECT) = -0.00115340367998
T1 (CC-PVQZ)= 0.012211651
T2 (CC-PVQZ)= 0.062674
E(HF/TZ-DKH) = -132.03211946
E(DLPNO-CCSDT/TZ-DKH) = -132.584903911
E(HF/CBS) = -131.987796106
E(DLPNO-CCSD(T)/CBS) = -132.586541671
E(DLPNO_TPNO/CC-PVTZ)) = -132.526451879
E(CV correction (DZ)) = -0.091092828506
E(CV correction (TZ)) = -0.147230666896
E(CV correction (CBS)) = -0.16698638142
E(TPNO_EFFECT) = -7.79412820009e-05
E(DKH correction) = -0.058529972875
E(HF/TZ-SMD) = -131.98569103
E(DLPNO-CCSDT/TZ-SMD) = -132.535983438749
dG(solv_DLPNO_SMD) = -0.00953156
E(HF/TZ-PCM) = -131.98568549
E(DLPNO-CCSDT/TZ-PCM) = -132.535983438749
dG(solv_DLPNO_PCM) = -0.00953156
E(PBE0/TZ-GAS) = -132.641529374
E(PBE0/TZ-SMD) = -132.652364643
dG(solv_PBE0_SMD) = -0.010835269295
E(B3LYP/6-31G(d)-GAS) = -132.670182052885
E(B3LYP/6-31G(d)-SMD) = -132.679699366697
dG(solv_B3LYP_6-31G(d)_SMD) = -0.00951731
dGcorr (HO): 0.0216657100
dGcorr(HO(100)): 0.0216657100
dGcorr(qRRHO): 0.0224474700

 C    -0.000004     0.000014    -0.487036
 H     0.000000     1.024412    -0.862033
 H    -0.887158    -0.512209    -0.862012
 H     0.887158    -0.512209    -0.861994
 C    -0.000005     0.000010     0.962059
 N     0.000009    -0.000019     2.111016
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$Na^+(MeCN)_4$

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Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -689.72435359
E(DLPNO-CCSD(T)/CC-PVTZ) = -692.194200301
T1 (CC-PVTZ)= 0.011674909
T2 (CC-PVTZ)= 0.060809
E(HF/CC-PVQZ) = -689.75842982
E(DLPNO-CCSD(T)/CC-PVQZ) = -692.383140576
E(HF/DZ-CORE) = -689.58884591
E(DLPNO-CCSD(T)/DZ-CORE) = -691.936425024
E(HF/DZ-CORE (FC)) = -689.58884591
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -
691.571691778
E(HF/TZ-CORE) = -689.72935111
E(DLPNO-CCSD(T)/TZ-CORE) = -692.815638974
E(HF/TZ-CORE (FC)) = -689.72935111
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -
692.226635816
E(HF/TZ-IT) = -689.72435359
E(DLPNO-CCSD(T)/TZ-IT) = -692.198903015
E(IT_EFFECT) = -0.00470271348104
T1 (CC-PVQZ)= 0.011676184
T2 (CC-PVQZ)= 0.062361
E(HF/TZ-DKH) = -690.16655108
E(DLPNO-CCSDT/TZ-DKH) = -692.637418798
E(HF/CBS) = -689.778097375
E(DLPNO-CCSD(T)/CBS) = -692.492189999
E(DLPNO_TPNO/CC-PVTZ)) = -692.193430904
E(CV correction (DZ)) = -0.364733246201
E(CV correction (TZ)) = -0.589003158029
E(CV correction (CBS)) = -0.667926972721
E(TPNO_EFFECT) = 0.000769397075032
E(DKH correction) = -0.443218497079
E(HF/TZ-SMD) = -689.79784988
E(DLPNO-CCSDT/TZ-SMD) = -692.261576837779
dG(solv_DLPNO_SMD) = -0.06814593
E(HF/TZ-PCM) = -689.78987311
E(DLPNO-CCSDT/TZ-PCM) = -692.261576837779
dG(solv_DLPNO_PCM) = -0.06814593
E(PBE0/TZ-GAS) = -692.701170993
E(PBE0/TZ-SMD) = -692.772080973
dG(solv_PBE0_SMD) = -0.0709099805871
E(B3LYP/6-31G(d)-GAS) = -692.8917386052
E(B3LYP/6-31G(d)-SMD) = -692.960709740448
dG(solv_B3LYP_6-31G(d)_SMD) = -0.06897114
dGcorr (HO): 0.1183531800
dGcorr(HO(100)): 0.1360851600
dGcorr(qRRHO): 0.1345755200

Na     0.015758    -0.008424    -0.036104
 C     1.662455     3.546487     3.018407
 H     1.912900     3.118416     3.990112
 H     0.887128     4.302467     3.150724
 H     2.551360     4.017572     2.596440
 C     1.189247     2.507349     2.131998
 N     0.813679     1.682005     1.429494
 C    -1.177147     1.980332    -4.434721
 H    -0.298648     2.442170    -4.887522
 H    -1.947019     2.740316    -4.293825
 H    -1.557673     1.206969    -5.103424
 C    -0.823582     1.397616    -3.160014
 N    -0.542952     0.935809    -2.148203
 C    -4.021088    -2.031450     2.034733
 H    -4.786845    -1.266225     2.169587
 H    -3.766406    -2.456506     3.006645
 H    -4.414909    -2.820557     1.392583
 C    -2.844682    -1.448144     1.430467
 N    -1.910850    -0.985546     0.950990
 C     3.522194    -3.483019    -0.602595
 H     4.423108    -3.036643    -1.025881
 H     3.165533    -4.267792    -1.271174
 H     3.763099    -3.922204     0.366530
 C     2.501483    -2.472244    -0.443131
 N     1.691266    -1.670229    -0.315901
```

$Na^+(MeCN)_5$

```
Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -821.70843419
E(DLPNO-CCSD(T)/CC-PVTZ) = -824.73806039
T1 (CC-PVTZ)= 0.011722191
T2 (CC-PVTZ)= 0.061605
E(HF/CC-PVQZ) = -821.75070664
E(DLPNO-CCSD(T)/CC-PVQZ) = -824.963980774
```

```
E(HF/DZ-CORE) = -821.54064199
E(DLPNO-CCSD(T)/DZ-CORE) = -824.454021832
E(HF/DZ-CORE (FC)) = -821.54064199
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -
823.998154918
E(HF/TZ-CORE) = -821.71468984
E(DLPNO-CCSD(T)/TZ-CORE) = -825.51417291
E(HF/TZ-CORE (FC)) = -821.71468984
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -
824.778025533
E(HF/TZ-IT) = -821.70843419
E(DLPNO-CCSD(T)/TZ-IT) = -824.743918927
E(IT_EFFECT) = -0.00585853639097
T1 (CC-PVQZ)= 0.011728301
T2 (CC-PVQZ)= 0.062708
E(HF/TZ-DKH) = -822.20897391
E(DLPNO-CCSDT/TZ-DKH) = -825.239803296
E(HF/CBS) = -821.775104754
E(DLPNO-CCSD(T)/CBS) = -825.094373765
E(DLPNO_TPNO/CC-PVTZ)) = -824.73656511
E(CV correction (DZ)) = -0.455866913792
E(CV correction (TZ)) = -0.73614737701
E(CV correction (CBS)) = -0.834782112095
E(TPNO_EFFECT) = 0.00149528024599
E(DKH correction) = -0.501742905625
E(HF/TZ-SMD) = -821.78872947
E(DLPNO-CCSDT/TZ-SMD) = -824.808912210459
dG(solv_DLPNO_SMD) = -0.07234710
E(HF/TZ-PCM) = -821.77897058
E(DLPNO-CCSDT/TZ-PCM) = -824.808912210459
dG(solv_DLPNO_PCM) = -0.07234710
E(PBE0/TZ-GAS) = -825.354600357
E(PBE0/TZ-SMD) = -825.431022936
dG(solv_PBE0_SMD) = -0.0764225786661
E(B3LYP/6-31G(d)-GAS) = -825.5756778027
E(B3LYP/6-31G(d)-SMD) = -825.649377456028
dG(solv_B3LYP_6-31G(d)_SMD) = -0.07369965
dGcorr (HO): 0.1531790700
dGcorr(HO(100)): 0.1733308100
dGcorr(qRRHO): 0.1727193400
```

Na	0.028735	-0.118941	-0.079985
C	-0.088817	1.786423	-4.748016
H	0.709844	2.519861	-4.866612
H	-1.048162	2.275415	-4.922385
H	0.044820	0.993708	-5.485351
C	-0.053668	1.229828	-3.413185
N	-0.025679	0.788912	-2.354507
C	0.482332	-3.583257	3.556175
H	-0.430168	-3.616307	4.152934
H	1.321281	-3.327906	4.204886
H	0.657409	-4.567821	3.120409
C	0.350817	-2.595695	2.507255
N	0.246613	-1.812430	1.675613
C	5.054833	-0.157762	-0.438670
H	5.496778	-0.124786	0.558061
H	5.394567	0.709583	-1.006233
H	5.386922	-1.065349	-0.944552
C	3.611678	-0.148562	-0.339199
N	2.467283	-0.141437	-0.260041
C	-0.881557	3.991089	2.629822
H	-1.632697	4.603122	2.128735
H	0.033667	4.573645	2.743247
H	-1.250906	3.713366	3.617912
C	-0.615404	2.801872	1.850835
N	-0.404354	1.858889	1.232785
C	-4.588807	-1.943921	-0.936005
H	-5.109319	-2.087555	0.011788
H	-4.523447	-2.901707	-1.453981
H	-5.158051	-1.245767	-1.551127
C	-3.261386	-1.421494	-0.695787
N	-2.208774	-1.007277	-0.505003

$Na^+(MeCN)_6$

```
Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -953.68979238
E(DLPNO-CCSD(T)/CC-PVTZ) = -957.279387111
T1 (CC-PVTZ)= 0.011744879
T2 (CC-PVTZ)= 0.061849
E(HF/CC-PVQZ) = -953.74023896
E(DLPNO-CCSD(T)/CC-PVQZ) = -957.541844777
E(HF/DZ-CORE) = -953.48973575
E(DLPNO-CCSD(T)/DZ-CORE) = -956.969435761
E(HF/DZ-CORE (FC)) = -953.48973575
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -
956.422418487
E(HF/TZ-CORE) = -953.69730791
E(DLPNO-CCSD(T)/TZ-CORE) = -958.210003354
E(HF/TZ-CORE (FC)) = -953.69730791
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -
957.326713496
E(HF/TZ-IT) = -953.68979238
E(DLPNO-CCSD(T)/TZ-IT) = -957.286400398
E(IT_EFFECT) = -0.00701328732998
T1 (CC-PVQZ)= 0.011761435
T2 (CC-PVQZ)= 0.062932
E(HF/TZ-DKH) = -954.24867951
E(DLPNO-CCSDT/TZ-DKH) = -957.839661543
E(HF/CBS) = -953.769354883
E(DLPNO-CCSD(T)/CBS) = -957.693325752
E(DLPNO_TPNO/CC-PVTZ)) = -957.277044974
E(CV correction (DZ)) = -0.547017274176
E(CV correction (TZ)) = -0.883289857503
E(CV correction (CBS)) = -1.00162902675
E(TPNO_EFFECT) = 0.00234213753595
E(DKH correction) = -0.56027443233
E(HF/TZ-SMD) = -953.77983044
E(DLPNO-CCSDT/TZ-SMD) = -957.356257415302
dG(solv_DLPNO_SMD) = -0.07921244
E(HF/TZ-PCM) = -953.76775993
E(DLPNO-CCSDT/TZ-PCM) = -957.356257415302
dG(solv_DLPNO_PCM) = -0.07921244
E(PBE0/TZ-GAS) = -958.005108952
E(PBE0/TZ-SMD) = -958.089813251
dG(solv_PBE0_SMD) = -0.0847042986769
E(B3LYP/6-31G(d)-GAS) = -958.2568220457
E(B3LYP/6-31G(d)-SMD) = -958.337983488799
dG(solv_B3LYP_6-31G(d)_SMD) = -0.08116144
dGcorr (HO): 0.1839713800
dGcorr(HO(100)): 0.2124409200
dGcorr(qRRHO): 0.2101199200
```

Na	0.004363	-0.000999	0.001266
C	-3.991123	-3.139989	-0.060376
H	-4.478589	-3.144170	0.915473
H	-4.711466	-2.819671	-0.814293
H	-3.660211	-4.152631	-0.294891
C	-2.857432	-2.240250	-0.044240
N	-1.958385	-1.527859	-0.031575
C	1.096084	-1.517256	4.727177
H	0.432234	-2.332512	5.018035
H	2.128410	-1.865784	4.779396
H	0.966492	-0.689320	5.425479
C	0.787021	-1.083240	3.381352
N	0.541616	-0.739417	2.314841
C	-1.135295	1.465104	-4.730181
H	-2.166659	1.818115	-4.770101
H	-0.472815	2.272173	-5.045916

H	-1.022004	0.625211	-5.416948
C	-0.804902	1.051675	-3.382937
N	-0.543065	0.724447	-2.315083
C	3.982799	3.157612	0.092237
H	3.844919	3.900376	0.879156
H	4.903098	2.604647	0.284965
H	4.072167	3.670374	-0.866410
C	2.855618	2.250005	0.065287
N	1.961616	1.531490	0.044116
C	2.984682	-3.661746	-1.861013
H	2.417411	-4.587421	-1.967029
H	3.372174	-3.370231	-2.838105
H	3.823103	-3.836059	-1.185346
C	2.132780	-2.617178	-1.333941
N	1.456880	-1.789942	-0.915722
C	-2.945063	3.704285	1.828189
H	-2.740647	3.861962	2.888021
H	-2.745026	4.630461	1.287695
H	-3.997073	3.443273	1.705711
C	-2.107339	2.641415	1.314986
N	-1.442263	1.800064	0.907711

METHANOL SOLVENT

MeOH

```
Charge of molecule: 0
Multiplicity: 1
E(HF/CC-PVTZ) = -115.08940165
E(DLPNO-CCSD(T)/CC-PVTZ) = -115.550410608
T1 (CC-PVTZ)= 0.008116557
T2 (CC-PVTZ)= 0.042865
E(HF/CC-PVQZ) = -115.09891272
E(DLPNO-CCSD(T)/CC-PVQZ) = -115.588638079
E(HF/DZ-CORE) = -115.05012882
E(DLPNO-CCSD(T)/DZ-CORE) = -115.490204517
E(HF/DZ-CORE (FC)) = -115.05012882
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -
115.429079178
E(HF/TZ-CORE) = -115.08990964
E(DLPNO-CCSD(T)/TZ-CORE) = -115.658470532
E(HF/TZ-CORE (FC)) = -115.08990964
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -
115.557455945
E(HF/TZ-IT) = -115.08940165
E(DLPNO-CCSD(T)/TZ-IT) = -115.550895745
E(IT_EFFECT) = -0.000485136592999
T1 (CC-PVQZ)= 0.008503808
T2 (CC-PVQZ)= 0.047466
E(HF/TZ-DKH) = -115.155669
E(DLPNO-CCSDT/TZ-DKH) = -115.616917626
E(HF/CBS) = -115.104402162
E(DLPNO-CCSD(T)/CBS) = -115.610701579
E(DLPNO_TPNO/CC-PVTZ)) = -115.550424778
E(CV correction (DZ)) = -0.061125338586
E(CV correction (TZ)) = -0.101014587284
E(CV correction (CBS)) = -0.115052188881
E(TPNO_EFFECT) = -1.41701919887e-05
E(DKH correction) = -0.066507017611
E(HF/TZ-SMD) = -115.09821098
E(DLPNO-CCSDT/TZ-SMD) = -115.558026871865
dG(solv_DLPNO_SMD) = -0.00760209
E(HF/TZ-PCM) = -115.09684344
E(DLPNO-CCSDT/TZ-PCM) = -115.557116723895
dG(solv_DLPNO_PCM) = -0.00669195
E(PBE0/TZ-GAS) = -115.637434451
E(PBE0/TZ-SMD) = -115.645680804
dG(solv_PBE0_SMD) = -0.00824635235999
E(B3LYP/6-31G(d)-GAS) = -115.645849013789
E(B3LYP/6-31G(d)-SMD) = -115.653983646641
dG(solv_B3LYP_6-31G(d)_SMD) = -0.00813463
dGcorr (HO): 0.0277608900
dGcorr(HO(100)): 0.0277608900
dGcorr(qRRHO): 0.0286406200
```

C	0.714948	0.015209	-0.000002
H	1.104730	0.522954	0.890935
H	1.093099	-1.007413	0.000415
H	1.104636	0.522198	-0.891411
O	-0.691841	-0.064583	0.000103
H	-1.047161	0.826329	-0.000105

$Na^{+}(MeOH)_4$

```
Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -622.16732061
E(DLPNO-CCSD(T)/CC-PVTZ) = -624.278472652
T1 (CC-PVTZ)= 0.008041743
T2 (CC-PVTZ)= 0.041928
E(HF/CC-PVQZ) = -622.20130858
E(DLPNO-CCSD(T)/CC-PVQZ) = -624.46364659
E(HF/DZ-CORE) = -622.02539361
E(DLPNO-CCSD(T)/DZ-CORE) = -623.906279076
E(HF/DZ-CORE (FC)) = -622.02539361
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -
623.661662634
E(HF/TZ-CORE) = -622.16928406
E(DLPNO-CCSD(T)/TZ-CORE) = -624.710145535
E(HF/TZ-CORE (FC)) = -622.16928406
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -
624.306047986
E(HF/TZ-IT) = -622.16732061
E(DLPNO-CCSD(T)/TZ-IT) = -624.280536089
E(IT_EFFECT) = -0.00206343746993
T1 (CC-PVQZ)= 0.008074099
T2 (CC-PVQZ)= 0.046594
E(HF/TZ-DKH) = -622.64117327
E(DLPNO-CCSDT/TZ-DKH) = -624.753501185
E(HF/CBS) = -622.220925194
E(DLPNO-CCSD(T)/CBS) = -624.570522222
E(DLPNO_TPNO/CC-PVTZ)) = -624.278504445
E(CV correction (DZ)) = -0.244616442104
E(CV correction (TZ)) = -0.404097549216
E(CV correction (CBS)) = -0.460221249635
E(TPNO_EFFECT) = -3.17930299616e-05
E(DKH correction) = -0.475028533712
E(HF/TZ-SMD) = -622.24745735
E(DLPNO-CCSDT/TZ-SMD) = -624.358226179148
dG(solv_DLPNO_SMD) = -0.07972173
E(HF/TZ-PCM) = -622.241093
E(DLPNO-CCSDT/TZ-PCM) = -624.352177503063
dG(solv_DLPNO_PCM) = -0.07367306
E(PBE0/TZ-GAS) = -624.678945103
E(PBE0/TZ-SMD) = -624.759670889
dG(solv_PBE0_SMD) = -0.0807257858399
E(B3LYP/6-31G(d)-GAS) = -624.7849840419
E(B3LYP/6-31G(d)-SMD) = -624.865348708878
dG(solv_B3LYP_6-31G(d)_SMD) = -0.08036467
dGcorr (HO): 0.1535963900
dGcorr(HO(100)): 0.1626800100
dGcorr(qRRHO): 0.1650906800
```

Na	-0.593875	0.047453	-0.216135
O	1.274882	-0.165073	-1.529924
H	1.449349	0.264714	-2.370686

C	2.414832	-0.944095	-1.171492
H	2.194594	-1.411306	-0.212506
H	3.303594	-0.318139	-1.062673
H	2.608085	-1.725884	-1.909593
O	-1.895313	-1.718923	-0.820742
H	-2.798386	-1.895438	-0.546698
C	-1.471459	-2.763399	-1.695564
H	-0.462164	-2.515779	-2.022031
H	-2.117971	-2.829469	-2.573344
H	-1.452041	-3.726412	-1.180363
O	-1.716860	2.025314	-0.074649
H	-2.256011	2.439111	-0.752835
C	-1.717977	2.863239	1.080493
H	-1.124931	2.357717	1.841418
H	-2.731047	3.007306	1.462366
H	-1.265602	3.833812	0.864613
O	0.514251	-0.018336	1.793406
H	0.309088	-0.560517	2.558947
C	1.660310	0.777346	2.090165
H	1.877892	1.371117	1.203021
H	2.527967	0.153559	2.316996
H	1.468793	1.452083	2.927808

$Na^+(MeOH)_5$

Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -737.27473097
E(DLPNO-CCSD(T)/CC-PVTZ) = -739.855094548
T1 (CC-PVTZ)= 0.008172690
T2 (CC-PVTZ)= 0.045096
E(HF/CC-PVQZ) = -737.31687148
E(DLPNO-CCSD(T)/CC-PVQZ) = -740.076838714
E(HF/DZ-CORE) = -737.098599
E(DLPNO-CCSD(T)/DZ-CORE) = -739.426607231
E(HF/DZ-CORE (FC)) = -737.098599
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -739.120914064
E(HF/TZ-CORE) = -737.27718228
E(DLPNO-CCSD(T)/TZ-CORE) = -740.394704345
E(HF/TZ-CORE (FC)) = -737.27718228
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -739.889640541
E(HF/TZ-IT) = -737.27473097
E(DLPNO-CCSD(T)/TZ-IT) = -739.85769073
E(IT_EFFECT) = -0.00259618152393
T1 (CC-PVQZ)= 0.008234059
T2 (CC-PVQZ)= 0.047880
E(HF/TZ-DKH) = -737.81481583
E(DLPNO-CCSDT/TZ-DKH) = -740.39658487
E(HF/CBS) = -737.341193443
E(DLPNO-CCSD(T)/CBS) = -740.204821345
E(DLPNO_TPNO/CC-PVTZ)) = -739.85517821
E(CV correction (DZ)) = -0.305693166908
E(CV correction (TZ)) = -0.505063803738
E(CV correction (CBS)) = -0.57522520465
E(TPNO_EFFECT) = -8.3661519966e-05
E(DKH correction) = -0.541490321535
E(HF/TZ-SMD) = -737.34888429
E(DLPNO-CCSDT/TZ-SMD) = -739.928907495583
dG(solv_DLPNO_SMD) = -0.07372929
E(HF/TZ-PCM) = -737.34401497
E(DLPNO-CCSDT/TZ-PCM) = -739.924343951952
dG(solv_DLPNO_PCM) = -0.06916574
E(PBE0/TZ-GAS) = -740.344145778
E(PBE0/TZ-SMD) = -740.418941491
dG(solv_PBE0_SMD) = -0.07479571339
E(B3LYP/6-31G(d)-GAS) = -740.4605384162
E(B3LYP/6-31G(d)-SMD) = -740.535222469253
dG(solv_B3LYP_6-31G(d)_SMD) = -0.07468405
dGcorr (HO): 0.2016814600
dGcorr(HO(100)): 0.2114895400
dGcorr(qRRHO): 0.2150204500

Na	0.682082	0.159923	-1.034111
O	-1.108935	1.203153	-0.083437
H	-1.491110	0.710238	0.660224
C	-1.702941	2.489771	-0.157210
H	-1.278666	3.002177	-1.020291
H	-2.785979	2.422435	-0.292996
H	-1.489153	3.082305	0.736723
O	0.474706	-1.463996	0.560778
H	-0.278931	-1.322481	1.155532
C	0.954466	-2.791348	0.708380
H	1.809878	-2.910076	0.043713
H	1.283270	-2.985062	1.733064
H	0.194422	-3.526543	0.429401
O	-1.787576	-0.574744	1.994817
H	-2.606362	-1.074961	1.928164
C	-1.613611	-0.140818	3.347499
H	-0.682048	0.421462	3.380597
H	-2.434466	0.508282	3.658335
H	-1.540608	-0.993505	4.025181
O	-0.017807	0.067623	-3.205971
H	0.482968	-0.158634	-3.992948
C	-1.375269	0.296886	-3.578398
H	-1.918499	0.533965	-2.664667
H	-1.458573	1.139016	-4.269546
H	-1.816624	-0.593670	-4.031928
O	2.902949	0.638373	-0.830573
H	3.471399	1.148880	-1.411537
C	3.650081	0.258580	0.323383
H	2.976066	-0.308086	0.964515
H	4.498808	-0.374185	0.053406
H	4.006065	1.135038	0.869902

$Na^+(MeOH)_6$

Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -852.36974766
E(DLPNO-CCSD(T)/CC-PVTZ) = -855.422850359
T1 (CC-PVTZ)= 0.008169749
T2 (CC-PVTZ)= 0.042526
E(HF/CC-PVQZ) = -852.41961595
E(DLPNO-CCSD(T)/CC-PVQZ) = -855.680442007
E(HF/DZ-CORE) = -852.15713629
E(DLPNO-CCSD(T)/DZ-CORE) = -854.936966497
E(HF/DZ-CORE (FC)) = -852.15713629
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -854.570135879
E(HF/TZ-CORE) = -852.37273344
E(DLPNO-CCSD(T)/TZ-CORE) = -856.069461114
E(HF/TZ-CORE (FC)) = -852.37273344
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -855.463550567
E(HF/TZ-IT) = -852.36974766
E(DLPNO-CCSD(T)/TZ-IT) = -855.425916138
E(IT_EFFECT) = -0.00306577859999
T1 (CC-PVQZ)= 0.008266630
T2 (CC-PVQZ)= 0.046682
E(HF/TZ-DKH) = -852.97612446
E(DLPNO-CCSDT/TZ-DKH) = -856.030836123
E(HF/CBS) = -852.448398105
E(DLPNO-CCSD(T)/CBS) = -855.829114493
E(DLPNO_TPNO/CC-PVTZ)) = -855.42231031
E(CV correction (DZ)) = -0.366830617543
E(CV correction (TZ)) = -0.605910547201

E(CV correction (CBS)) = -0.690046220645
E(TPNO_EFFECT) = 0.000540049429105
E(DKH correction) = -0.607985763531
E(HF/TZ-SMD) = -852.45509245
E(DLPNO-CCSDT/TZ-SMD) = -855.506295586174
dG(solv_DLPNO_SMD) = -0.08398528
E(HF/TZ-PCM) = -852.4426518
E(DLPNO-CCSDT/TZ-PCM) = -855.494952488577
dG(solv_DLPNO_PCM) = -0.07264218
E(PBE0/TZ-GAS) = -855.995293106
E(PBE0/TZ-SMD) = -856.080981793
dG(solv_PBE0_SMD) = -0.085688687419
E(B3LYP/6-31G(d)-GAS) = -856.1093169942
E(B3LYP/6-31G(d)-SMD) = -856.195978500805
dG(solv_B3LYP_6-31G(d)_SMD) = -0.08666151
dGcorr (HO): 0.2493440500
dGcorr(HO(100)): 0.2564938100
dGcorr(qRRHO): 0.2628954800

Na	0.000856	0.000645	0.000852
O	-0.485601	-2.259349	-0.622829
H	-0.803307	-2.612855	-1.456067
C	-0.317316	-3.335380	0.290667
H	0.044525	-2.903135	1.222003
H	-1.263028	-3.849892	0.482312
H	0.417581	-4.058755	-0.073319
O	-2.039575	0.844825	-0.922970
H	-2.450915	0.665943	-1.770901
C	-2.866437	1.747496	-0.200260
H	-2.374475	1.929033	0.753734
H	-2.978376	2.698569	-0.728206
H	-3.856338	1.322047	-0.013368
O	2.039704	-0.846300	0.923262
H	2.451334	-0.667883	1.771153
C	2.865963	-1.749073	0.200004
H	2.374235	-1.929163	-0.754382
H	3.856367	-1.324429	0.013954
H	2.976723	-2.700780	0.727058
O	-1.239161	-0.421915	1.994818
H	-1.018613	-0.227302	2.907875
C	-2.507467	-1.063015	1.962381
H	-2.726905	-1.272464	0.916894
H	-2.494434	-2.005059	2.517544
H	-3.292520	-0.418414	2.367335
O	1.241991	0.422808	-1.992796
H	1.022674	0.226927	-2.905879
C	2.510251	1.063979	-1.959533
H	2.728545	1.274417	-0.914001
H	3.295776	0.419014	-2.362981
H	2.497818	2.005491	-2.515609
O	0.483671	2.262158	0.623230
H	0.798152	2.619245	1.456164
C	0.314888	3.334908	-0.294083
H	-0.044007	2.898943	-1.224815
H	-0.422419	4.057751	0.066064
H	1.259844	3.850961	-0.485304

E(HF/CC-PVQZ) = -161.67672776
E(DLPNO-CCSD(T)/CC-PVQZ) = -161.970093902
E(HF/DZ-CORE) = -161.67110379
E(DLPNO-CCSD(T)/DZ-CORE) = -161.775474796
E(HF/DZ-CORE (FC)) = -161.67110379
E(DLPNO-CCSD(T)/DZ-CORE (FC)) = -161.775474796
E(HF/TZ-CORE) = -161.67602684
E(DLPNO-CCSD(T)/TZ-CORE) = -161.930995713
E(HF/TZ-CORE (FC)) = -161.67602684
E(DLPNO-CCSD(T)/TZ-CORE (FC)) = -161.930995713
E(HF/TZ-IT) = -161.67602684
E(DLPNO-CCSD(T)/TZ-IT) = -161.931112215
E(IT_EFFECT) = -8.86592810048e-05
T1 (CC-PVQZ)= 0.003567893
T2 (CC-PVQZ)= 0.013921
E(HF/TZ-DKH) = -161.88486023
E(DLPNO-CCSDT/TZ-DKH) = -162.140136008
E(HF/CBS) = -161.677132305
E(DLPNO-CCSD(T)/CBS) = -161.992643878
E(DLPNO_TPNO/CC-PVTZ)) = -161.930995713
E(CV correction (DZ)) = 0.0
E(CV correction (TZ)) = 0.0
E(CV correction (CBS)) = -0.0
E(TPNO_EFFECT) = 2.78426059879e-05
E(DKH correction) = -0.209112451729
dGcorr: -0.0144286900

Na	0.000000	0.000000	0.000000

SODIUM CATION (GAS)

Na^+

Charge of molecule: 1
Multiplicity: 1
E(HF/CC-PVTZ) = -161.67602684
E(DLPNO-CCSD(T)/CC-PVTZ) = -161.931023556
T1 (CC-PVTZ)= 0.004410652
T2 (CC-PVTZ)= 0.018894