Supplementary data for "Symmetric versus asymmetric discretization of the integral equations in polarizable continuum solvation models"

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This document provides some additional numerical data that augment the results in the paper. In addition, we provide the atomic coordinates for each of the molecules in our data set, along with the atomic radii that are used to construct the solute cavities.

1 Additional data

In Section II A of the paper, we discussed the general matrix formulation of PCMs in terms of Eq. 7. We present the corresponding **K** and **R** matrices for C-PCM and IEF-PCM in Table S1, where the **K**-matrix variants considered in this work are explicitly shown.

In Section IV A of the paper, we discuss the differences in the total energy, W, between the symmetric and asymmetric forms of **K** for the amino acids in water. For the data shown in Fig. 1 of the paper, cavity surfaces were discretized using $N = 590$ Lebedev points per

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Method	Matrix **K**	Matrix **R**
C-PCM	$\mathbf{S}$	$-[(\varepsilon-1)/\varepsilon]\mathbf{I}$
IEF-PCM ($\mathbf{X} = \mathbf{DAS}$ form)	$\mathbf{S} - (f_\varepsilon/2\pi)\mathbf{DAS}$	$-f_\varepsilon\mathbf{Y}$
IEF-PCM ($\mathbf{X} = \mathbf{SAD}^\dagger$ form)	$\mathbf{S} - (f_\varepsilon/2\pi)\mathbf{SAD}^\dagger$	$-f_\varepsilon\mathbf{Y}$
IEF-PCM (symmetric form)	$\mathbf{S} - (f_\varepsilon/4\pi)(\mathbf{SAD} + \mathbf{SAD}^\dagger)$	$-f_\varepsilon\mathbf{Y}$

Table S1: Possible definitions for the matrices **K** and **R** in Eq. (7).

atomic sphere, but we have performed the same calculations using $N = 50$ and $N = 110$ as well. Figure S1 below shows the energy differences that we obtain using $N = 110$. (This figure is the analogue of Fig. 1 in the paper, using a less dense grid.) We find that the denser grid can lead to even larger variations among the different forms of $\mathbf{K}$. We tests three different grid densities ($N = 50$, 110, and 590), and Table S2 shows the largest variations in energy, amongst the different forms of $\mathbf{K}$, that are obtained in each case, for a variety of discretization procedures as described in the paper.

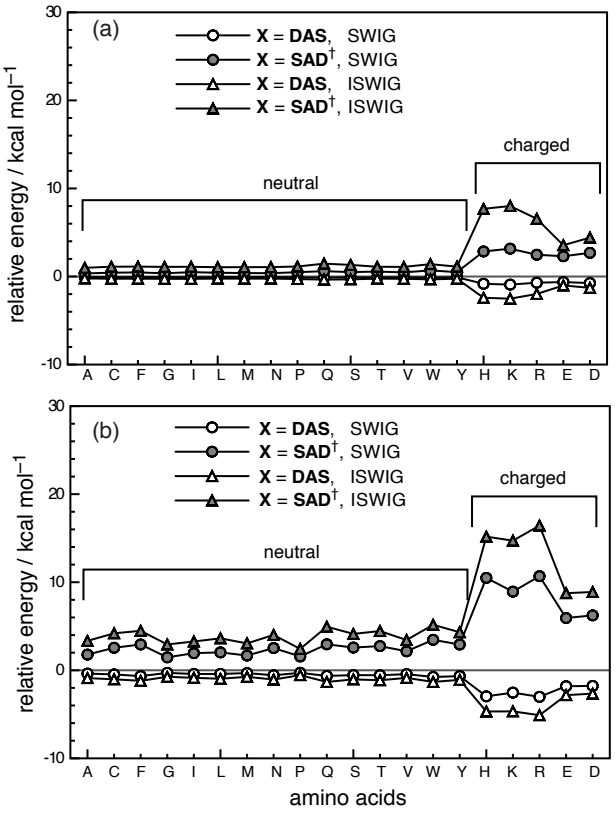

Figure S1: Relative energies of the amino acids in water ($\varepsilon = 78.39$), obtained at (a) the AMBER99 level and (b) the HF/6-31+G* level. The cavity surface was discretized using $N = 110$ Lebedev points per atomic sphere, and solution-phase energies are reported relative to the energy obtained using the symmetric form of $\mathbf{K}$.

AMBER99 solutes						
N	$\mathbf{X} = \mathbf{DAS}$			$\mathbf{X} = \mathbf{SAD}^\dagger$		
	GBO	ISWIG	SWIG	GBO	ISWIG	SWIG
50	−1.0	−0.6	−2.0	3.4	2.4	6.9
110	—	−0.9	−2.5	—	3.2	8.0
590	−1.0	−1.6	−2.8	3.2	4.6	7.7
HF/6-31+G* solutes						
N	$\mathbf{X} = \mathbf{DAS}$			$\mathbf{X} = \mathbf{SAD}^\dagger$		
	GBO	ISWIG	SWIG	GBO	ISWIG	SWIG
50	−3.1	−2.1	−4.5	9.7	8.8	15.4
110	—	−3.0	−5.1	—	10.7	16.4
590	−4.3	−5.0	−9.2	11.8	14.5	24.0

Table S2: Maximum (signed) difference, in kcal/mol, between the IEF-PCM energy computed using $\mathbf{X} = \mathbf{DAS}$ or $\mathbf{X} = \mathbf{SAD}^\dagger$, and that computed using the symmetric form of $\mathbf{X}$. The data set is the amino acids in water. Three different values of N, the number of Lebedev points per atomic sphere, and three different discretization procedures are compared.

In Fig. 2 of the text, we plot W for a variety of different discretization schemes, relative to the energy obtained using Gaussian blurring only (GBO). Effectively, we are taking GBO discretization as the benchmark, so here we assess the reliability of this benchmark. Figure S2 plots the energy difference $W_{\mathrm{GBO}} - W_{\mathrm{APBS}}$ for the aqueous amino acids, where W_{GBO} represents the IEF-PCM solvation energy computed using GBO discretization and W_{APBS} is the energy obtained using the adaptive Poisson-Boltzmann (APBS) software[1] to solve the three-dimensional Poisson-Boltzmann equation. The same solute cavity is used for both the APBS and the IEF-PCM calculations, and the solute is described at the AMBER99 level so that there is no escaped charge. The APBS calculations use a $193 \times 193 \times 193$ grid with a resolution of 0.1 Å, and appear to be converged with respect to the grid parameters. (These grid parameters are consistent with other benchmark APBS calculations.[2–4]) As such, W_{APBS} should be the *exact* solution-phase energy, since we consider only electrostatic contributions to the solvation energy. Using $\mathbf{X} = \mathbf{DAS}$, we find that $|W_{\mathrm{GBO}} - W_{\mathrm{APBS}}| < 0.13$ kcal/mol for the entire amino acid data set. This means that IEF-PCM with $\mathbf{X} = \mathbf{DAS}$ and GBO discretization is essentially exact (in the absence of escaped charge), which justifies the use of this method as a benchmark in Fig. 2 of the paper.

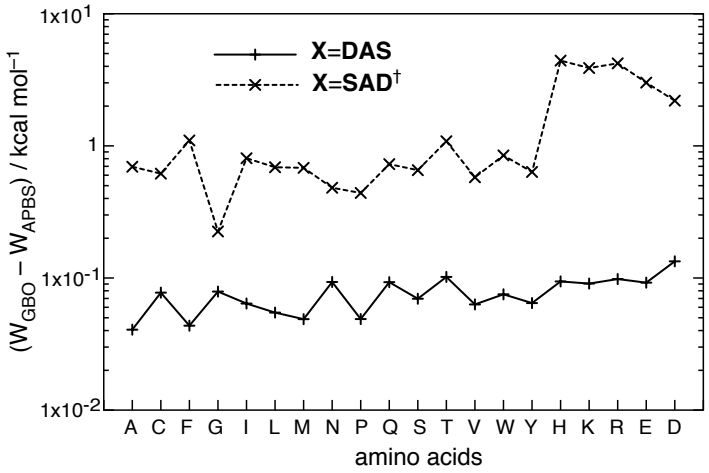

Figure S2: Comparison of total energies obtained for AMBER99 solutes, computed by numerical solution of the Poisson-Boltzmann equation (using the APBS software) to those obtained from two different forms of IEF-PCM with GBO discretization. The APBS and IEF-PCM solute cavities are identical. APBS calculations used a $193 \times 193 \times 193$ grid with a grid resolution of 0.1 Å, whereas IEF-PCM calculations used $N = 590$ Lebedev points per atomic sphere.

Section V B of the paper discusses the quadratic scaling of E_{pol} with respect to the electrostatic potential. This relationship is exact when a force field is used to represent the solute, but the same need not be true for a quantum-mechanical solute. We have tested this relationship using HF/6-31+G* calculations on a series of ionized histidine solutes, His^{n+}. Assuming that the solute's internal energy, E_0, is approximately the same regardless of whether the $\mathbf{X} = \mathbf{DAS}$ or $\mathbf{X} = \mathbf{SAD}^\dagger$ form of IEF-PCM is employed, and assuming furthermore that the electrostatic potential grows in proportion to the molecular charge, n, then based upon the analysis in Section V B one should expect the energy difference $W_{\text{DAS}} - W_{\text{SAD}^\dagger}$ to grow quadratically with n. Calculated values of $W_{\text{DAS}} - W_{\text{SAD}^\dagger}$ are plotted versus n in Fig. S3, and the quadratic dependence is evident. This demonstrates that the analysis in Section V B is likely to be valid even for quantum-mechanical solutes.

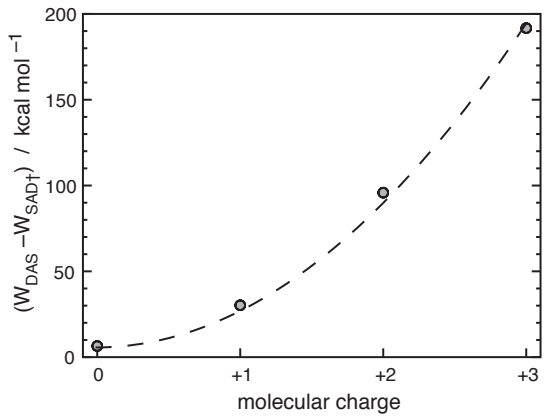

Figure S3: Difference in total energy between the $\mathbf{X} = \mathbf{SAD}^\dagger$ and $\mathbf{X} = \mathbf{DAS}$ forms of $\mathbf{K}$, for successive ionization of histidine described at the HF/6-31+G* level. (The dashed curve is a quadratic fit to the four data points.) The cavity surface is discretized with SWIG using $N = 590$ Lebedev points per atomic sphere, and $\varepsilon = 78.39$.

2 Comparison of FIXPVA implementations

As mentioned in the paper, our original implementation[5,6] of the FIXPVA discretization algorithm[7] differs slightly from Su and Li's original implementation in the GAMESS software,[8,9] owing to certain details of the switching functions that were omitted from the description of the algorithm in Ref. 7. Here, we present confirmation that our new implementation of FIXPVA is identical to that in GAMESS. Specifically, we compare the energy, surface area, and Gauss' law error (for the nuclear charges) that we obtain using our implementation (in a locally-modified version of Q-Chem[10]) to those obtained using GAMESS (version of 1 Oct. 2010). Consistent with the GAMESS implementation, both sets of calculations use GEPOL grids.[11–13] These grids were generated using GAMESS, then read into our Q-Chem code. To avoid complications in the definitions of $\mathbf{D}$ and $\mathbf{K}$, we carry out these calculations using the C-PCM solvation model, where the $\mathbf{D}$ matrix is absent and $\mathbf{K} \equiv \mathbf{S} = \mathbf{S}^\dagger$. We find that the total energies (at the HF/6-31+G*/C-PCM level) obtained using the Q-Chem and GAMESS implementations of FIXPVA differ by no more than 10^{-9} hartree.

A more interesting comparison is between FIXPVA calculations using GEPOL versus Lebedev grids, and we present such a comparison (again at the HF/6-31+G*/C-PCM level) in Table S3, where the data set is the amino acids in water ($\varepsilon = 78.39$), and solute cavities are constructed using Bondi radii[14] (except for hydrogen[15]), each scaled by a factor of 1.2.

Amino	GEPOL			Lebedev		
Acid	W/E_h	SA/Å^2	Δ_{Gauss}/e	W/E_h	SA/Å^2	Δ_{Gauss}/e
A	-321.88334	83.82	0.71	-321.88320	83.00	0.76
C	-719.38547	102.72	0.76	-719.38496	102.87	0.82
F	-551.43051	120.57	1.18	-551.43027	121.31	1.28
G	-282.84839	74.18	0.57	-282.84827	75.07	0.57
I	-438.96596	102.45	1.12	-438.96556	101.11	1.27
L	-438.90410	102.37	1.15	-438.90354	100.68	1.35
M	-797.45500	121.21	1.03	-797.45490	121.77	1.07
N	-489.62292	101.99	0.92	-489.62244	101.07	1.02
P	-398.77831	92.77	0.98	-398.77769	91.92	1.11
Q	-528.69266	113.56	1.06	-528.69229	113.95	1.10
S	-396.73413	91.53	0.74	-396.73352	90.59	0.85
T	-435.76094	96.16	0.86	-435.75998	95.21	1.00
V	-399.94481	98.27	1.02	-399.94464	98.15	1.09
W	-682.17613	134.52	1.34	-682.17580	134.13	1.46
Y	-626.29219	130.31	1.22	-626.29207	131.13	1.28
H	-603.39912	123.95	1.46	-603.39848	123.88	1.57
K	-546.00669	112.63	1.15	-546.00601	112.00	1.30
R	-494.47461	108.82	1.35	-494.47405	110.25	1.41
E	-548.07604	115.23	0.97	-548.07566	116.19	1.01
D	-509.01129	105.27	0.80	-509.01070	103.79	0.91
Absolute Differences	W/kcal mol^{-1}	SA/Å^2	Δ_{Gauss}/e			
Average:	0.27	0.81	0.09			
RMS:	0.16	0.43	0.06			
Maximum:	0.60	1.69	0.20			

Table S3: Comparison of FIXPVA calculations (at the HF/6-31+G*/C-PCM level) carried out using either GEPOL grids (with 240 points per atom) or Lebedev grids (with 194 points per atom). Total energies (W), surface areas (SA), and Gauss' law errors (Δ_{Gauss}, for the nuclear charges only) are compared. The data set is the amino acids in water ($\varepsilon = 78.39$) and solute cavities are constructed using Bondi radii[14,15] scaled by 1.2 GEPOL calculations were carried out using GAMESS and Lebedev calculations were performed using our locally-modified version of Q-Chem.

Su and Li[7] report rotational variance errors of 0.9 and 0.2 kcal/mol, for FIXPVA calculations with GEPOL grids of 60 and 240 points per sphere, respectively. These errors are one metric tp characterize the quality of the integration grid, and they are comparable to the differences in W between GEPOL and Lebedev integration grids. As such, GEPOL and Lebedev grids appear to be of comparable quality, when the number of grid points per atom

is comparable. On average, surface areas agree within 1 Å^2, and the errors in Gauss' law error (for the nuclear charges) differ by only about $0.1e$. The use of denser grids should yield even better agreement between GEPOL and Lebedev grids. As the grid density increases, these differences become even smaller. (One advantage of Lebedev grids in this respect is that they are available for very large number of grid points per atom,[16] so that PCM calculations can be converged to the infinite-grid limit.) In any case, the differences between Lebedev and GEPOL grids that are documented in Table S3 are far smaller than the variations in W, SA, and Δ_{Gauss} that are engendered by the choice of the $\mathbf{K}$ matrix.

3 FIXPVA discontinuity

In Section V A of the paper, we noted that one of the FIXPVA switching functions may exhibit discontinuities if the radius of any atomic sphere is smaller than the n_2 parameter defined in Ref. 7. Here, we provide a numerical example. To do so, we plot the electrostatic solvation energy, E_{pol}, along with the total cavity surface area, for dissociation of NaCl at the HF/6-31G* level. In order to observe the discontinuity, we use radii of 1.2 Å and 1.4 Å for the Na and Cl, respectively, whereas the value $n_2 = 1.5$ Å is taken from Ref. 7. The calculation is carried out using GAMESS, and results are plotted in Fig. S4. It is clear that both E_{pol} and the cavity surface area are discontinuous functions of the internuclear distance; these discontinuities occur precisely where the internuclear distance equals an atomic radius.

Figure S4 serves only as a numerical illustration that discontinuities may occur in FIXPVA calculations. It is not intended to be a chemically realistic example, and indeed one may argue that the atomic radii used in this example are too small. On the other hand, once could easily conceive of other, more relevant examples where atomic radii (especially those belonging to hydrogen atoms) might fall below the n_2 threshold. Proton transfer along a hydrogen-bond coordinate, a cationic organic molecule, or a metal cation might all fall into this category of problematic examples.

4 Amino acid data set

Cartesian coordinates for the amino acids in our data set are reported here, in Angstrom units. We also provide the AMBER99 point charges, q_{AMBER}, along with the atomic radii that were used to construct the solute cavities. There are two such radii for each atom: R_{HF} (used for HF/6-31+G* solutes) and R_{AMBER} (used for AMBER99 solutes). The radius R_{HF} is

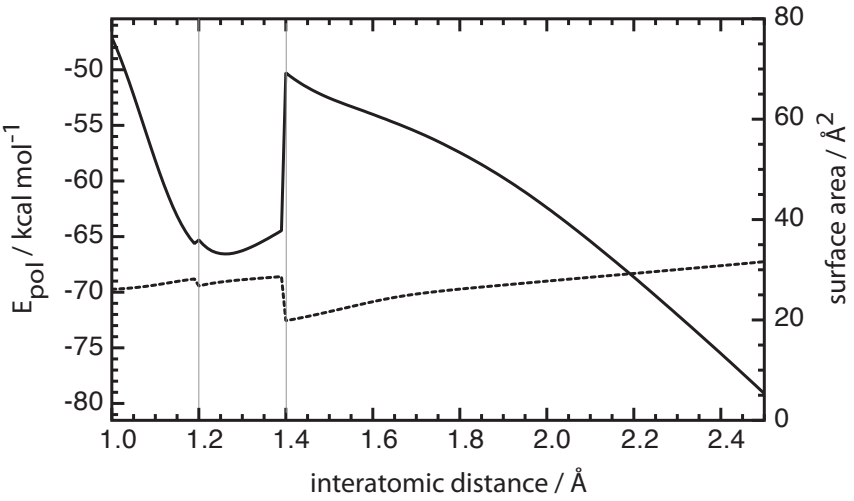

Figure S4: Illustration of FIXPVA discontinuity along Na–Cl dissociation at HF/6-31+G* level, using the GAMESS implementation of FIXPVA. The solid curve represents the electrostatic solvation energy, E_{pol}, and the dashed curve is the total cavity surface area. The calculation uses a GEPOL grid with 60 points per sphere. Discontinuities are observed when the internuclear distance equals 1.2 Å (the atomic radius used for Na) and 1.4 Å (the radius used for Cl); these are marked with broken vertical lines. Data points are spaced 0.01 Å apart.

the Bondi radius scaled by a factor of 1.2, whereas R_{AMBER} is the AMBER99 Lennard-Jones radius plus 1.4 Å. The additional 1.4 Å represents the "solvent probe" radius for water,[17] so the AMBER99 calculations use a "solvent-accessible surface".

The reader may notice that the charges q_{AMBER} do not always sum exactly to the expected total charge of each amino acid. The charges that we use are the default atomic charges produced by the TINKER program, version 4.2.

Alanine (A), charge = 0						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	0.000000	0.000000	0.000000	0.1414	3.2750	1.860
C	-0.939800	0.980143	0.637256	0.1281	3.3080	2.040
C	-0.206362	2.187874	1.169755	0.7731	3.3080	2.040
O	0.844057	1.975752	1.813281	-0.8055	3.0612	1.824
H	-0.390471	-0.318989	-0.886667	0.1997	2.0000	1.320
H	0.107996	-0.812362	0.607293	0.1997	2.0000	1.320
H	0.890045	0.458728	-0.194396	0.1997	2.0000	1.320
H	-1.674910	1.332233	-0.116234	0.0889	2.7870	1.320
C	-1.659858	0.307112	1.820534	-0.1825	3.3080	2.040
H	-2.354777	1.033764	2.290815	0.0603	2.8870	1.320
H	-0.909682	-0.023116	2.569057	0.0603	2.8870	1.320
H	-2.235041	-0.568037	1.452597	0.0603	2.8870	1.320
O	-0.705498	3.307775	0.926477	-0.8055	3.0612	1.824

Cysteine (C), charge = 0						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	0.000000	0.000000	-0.000000	0.1325	3.2750	1.860
C	-0.595955	-1.374805	-0.068916	0.0978	3.3080	2.040
C	-0.816222	-1.814240	-1.496669	0.7497	3.3080	2.040
O	-1.330682	-0.981280	-2.273849	-0.7981	3.0612	1.824
H	0.758910	0.008354	0.681458	0.2023	2.0000	1.320
H	-0.709710	0.663574	0.310454	0.2023	2.0000	1.320
H	0.390092	0.247969	-0.909252	0.2023	2.0000	1.320
H	0.093173	-2.101772	0.409334	0.1411	2.7870	1.320
C	-1.962527	-1.378884	0.641058	-0.1231	3.3080	2.040
S	-2.672875	-3.052026	0.549416	-0.3119	3.4000	2.160
H	-2.623656	-0.620226	0.172603	0.1112	2.7870	1.320
H	-1.834204	-1.038492	1.689755	0.1112	2.7870	1.320
H	-3.799169	-2.762680	1.215255	0.1933	2.0000	1.320
O	-0.467324	-2.977497	-1.792646	-0.7981	3.0612	1.824

Phenylalanine (F), charge = 0						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	0.000000	0.000000	0.000000	0.1737	3.2750	1.860
C	-0.394616	0.675463	-1.279855	0.0859	3.3080	2.040
C	-1.680664	1.451524	-1.125232	0.7660	3.3080	2.040
O	-2.617215	0.883671	-0.522807	-0.8026	3.0612	1.824
H	0.995911	0.143155	0.167533	0.1921	2.0000	1.320
H	-0.165208	-1.003383	-0.079563	0.1921	2.0000	1.320
H	-0.513345	0.416170	0.776968	0.1921	2.0000	1.320
H	0.400052	1.388857	-1.582629	0.1041	2.7870	1.320
C	-0.613575	-0.385249	-2.374636	-0.0343	3.3080	2.040
C	-1.008192	0.290214	-3.654491	0.0118	3.3080	2.040
C	-0.031736	0.687087	-4.560650	-0.1256	3.3080	2.040
C	-2.350326	0.519269	-3.934330	-0.1256	3.3080	2.040
C	-0.397413	1.313016	-5.746649	-0.1704	3.3080	2.040
C	-2.716004	1.145198	-5.120329	-0.1704	3.3080	2.040
C	-1.739547	1.542072	-6.026488	-0.1072	3.3080	2.040
H	-1.420866	-1.078939	-2.059712	0.0295	2.8870	1.320
H	0.327533	-0.952391	-2.532007	0.0295	2.8870	1.320
H	1.030384	0.505820	-4.339195	0.1330	2.8590	1.320
H	-3.123061	0.205197	-3.217225	0.1330	2.8590	1.320
H	0.375321	1.627088	-6.463753	0.1430	2.8590	1.320
H	-3.778124	1.326465	-5.341784	0.1430	2.8590	1.320
H	-2.028932	2.037411	-6.965048	0.1297	2.8590	1.320
O	-1.710760	2.602698	-1.611436	-0.8026	3.0612	1.824

Glycine (G), charge = 0						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	0.000000	0.000000	0.000000	0.2943	3.2750	1.860
C	0.628853	0.322341	-1.323118	-0.0100	3.3080	2.040
C	2.124342	0.491899	-1.201211	0.7231	3.3080	2.040
O	2.541498	1.177247	-0.242681	-0.7855	3.0612	1.824
H	-0.668980	-0.760983	-0.117345	0.1642	2.0000	1.320
H	-0.507309	0.815480	0.343556	0.1642	2.0000	1.320
H	0.719822	-0.310911	0.652374	0.1642	2.0000	1.320
H	0.436448	-0.506061	-2.036442	0.0895	2.7870	1.320
H	0.208207	1.273330	-1.711420	0.0895	2.7870	1.320
O	2.831258	-0.066003	-2.068112	-0.7855	3.0612	1.824

Isoleucine (I), charge = 0						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	-0.000000	0.000000	0.000000	0.0311	3.2750	1.860
C	-1.097827	-0.294094	0.978920	0.0389	3.3080	2.040
C	-2.429151	0.228560	0.494659	0.8343	3.3080	2.040
O	-2.446405	1.385165	0.020878	-0.8190	3.0612	1.824
H	0.577689	-0.831494	-0.123666	0.2329	2.0000	1.320
H	0.593176	0.744176	0.367076	0.2329	2.0000	1.320
H	-0.405653	0.239382	-0.904733	0.2329	2.0000	1.320
H	-1.190609	-1.392083	1.112761	0.1031	2.7870	1.320
C	-0.758741	0.344355	2.338700	0.1303	3.3080	2.040
C	-1.885844	0.042419	3.343725	-0.0430	3.3080	2.040
C	-0.615385	1.868316	2.169610	-0.3204	3.3080	2.040
C	-1.546758	0.680868	4.703505	-0.0660	3.3080	2.040
H	0.195424	-0.078377	2.716809	0.0187	2.8870	1.320
H	-1.985509	-1.056219	3.466850	0.0236	2.8870	1.320
H	-2.840009	0.465151	2.965616	0.0236	2.8870	1.320
H	0.195423	2.095434	1.446347	0.0882	2.8870	1.320
H	-0.370910	2.337241	3.145541	0.0882	2.8870	1.320
H	-1.566462	2.299688	1.793486	0.0882	2.8870	1.320
H	-2.354346	0.468180	5.434713	0.0186	2.8870	1.320
H	-1.441366	1.780117	4.591059	0.0186	2.8870	1.320
H	-0.591697	0.267348	5.089459	0.0186	2.8870	1.320
O	-3.412575	-0.535196	0.604450	-0.8190	3.0612	1.824

Leucine (L), charge = 0						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	-0.000000	0.000000	0.000000	0.1010	3.2750	1.860
C	-0.091798	-1.421308	-0.470592	0.0343	3.3080	2.040
C	-1.401891	-2.056103	-0.069606	0.8326	3.3080	2.040
O	-1.788101	-1.867485	1.104177	-0.8199	3.0612	1.824
H	0.358351	0.585883	-0.754139	0.2148	2.0000	1.320
H	0.652588	0.058352	0.781745	0.2148	2.0000	1.320
H	-0.930315	0.337756	0.246648	0.2148	2.0000	1.320
H	-0.023635	-1.450049	-1.578125	0.1053	2.7870	1.320
C	1.044248	-2.246588	0.161795	-0.1102	3.3080	2.040
C	0.950002	-3.705798	-0.321346	0.3531	3.3080	2.040
C	2.086047	-4.531077	0.311043	-0.4121	3.3080	2.040
C	-0.407840	-4.299352	0.097652	-0.4121	3.3080	2.040
H	0.949793	-2.217433	1.267385	0.0457	2.8870	1.320
H	2.022979	-1.820102	-0.142003	0.0457	2.8870	1.320
H	1.044456	-3.734952	-1.426935	-0.0361	2.8870	1.320
H	2.016559	-5.582392	-0.038254	0.1000	2.8870	1.320
H	1.990951	-4.502831	1.416600	0.1000	2.8870	1.320
H	3.064792	-4.105258	0.006353	0.1000	2.8870	1.320
H	-0.474001	-5.350975	-0.251360	0.1000	2.8870	1.320
H	-1.226632	-3.706509	-0.360844	0.1000	2.8870	1.320
H	-0.496789	-4.271676	1.203736	0.1000	2.8870	1.320
O	-2.000402	-2.721857	-0.941991	-0.8199	3.0612	1.824

Methionine (M), charge = 0						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	0.000000	0.000000	0.000000	0.1592	3.2750	1.860
C	1.499698	0.025928	0.015289	0.0429	3.3080	2.040
C	2.027427	1.166047	0.852982	0.8013	3.3080	2.040
O	1.486273	2.282106	0.697853	-0.8105	3.0612	1.824
H	-0.325458	-0.956316	0.141197	0.1984	2.0000	1.320
H	-0.336754	0.316540	-0.909285	0.1984	2.0000	1.320
H	-0.358229	0.571116	0.765440	0.1984	2.0000	1.320
H	1.882259	-0.921570	0.448875	0.1116	2.7870	1.320
C	2.025250	0.213747	-1.420022	0.0342	3.3080	2.040
C	3.564940	0.240367	-1.404325	0.0018	3.3080	2.040
S	4.171098	0.462723	-3.105951	-0.2737	3.4000	2.160
C	5.943017	0.444093	-2.690797	-0.0536	3.3080	2.040
H	1.644081	1.172362	-1.829740	0.0241	2.8870	1.320
H	1.677503	-0.629002	-2.053223	0.0241	2.8870	1.320
H	3.945244	-0.696601	-0.946548	0.0440	2.7870	1.320
H	3.912832	1.050371	-0.729813	0.0440	2.7870	1.320
H	6.582078	0.567501	-3.589948	0.0684	2.7870	1.320
H	6.234935	-0.483432	-2.155465	0.0684	2.7870	1.320
H	6.203279	1.222771	-1.943788	0.0684	2.7870	1.320
O	2.965243	0.906948	1.637756	-0.8105	3.0612	1.824

Asparagine (N), charge = 0						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	0.000000	0.000000	0.000000	0.1801	3.2750	1.860
C	0.783232	-1.274109	0.114866	0.0811	3.3080	2.040
C	1.076420	-1.618414	1.555558	0.8050	3.3080	2.040
O	1.476527	-0.690054	2.290788	-0.8147	3.0612	1.824
H	-0.759042	-0.126122	-0.669588	0.1921	2.0000	1.320
H	0.606811	0.742536	-0.347593	0.1921	2.0000	1.320
H	-0.412316	0.228923	0.904428	0.1921	2.0000	1.320
H	0.198182	-2.109475	-0.323293	0.1231	2.7870	1.320
C	2.130102	-1.117165	-0.615140	-0.2041	3.3080	2.040
C	2.884929	-2.417521	-0.475818	0.7130	3.3080	2.040
O	3.992611	-2.587394	-0.958086	-0.5931	3.0612	1.824
N	2.131403	-3.400644	0.035322	-0.9191	3.2240	1.860
H	2.726595	-0.321846	-0.121413	0.0797	2.8870	1.320
H	1.945696	-0.943833	-1.695904	0.0797	2.8870	1.320
H	1.160076	-3.204481	0.277075	0.4196	2.0000	1.320
H	2.589302	-4.235598	0.400809	0.4196	2.0000	1.320
O	0.896684	-2.805567	1.903212	-0.8147	3.0612	1.824

Proline (P), charge = 0						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	0.000000	-0.000000	0.000000	-0.2020	3.2750	1.860
C	0.619225	-1.274972	0.490923	0.1589	3.3080	2.040
C	-0.429094	-2.307429	0.830272	0.6631	3.3080	2.040
O	-1.416964	-1.917650	1.489580	-0.7697	3.0612	1.824
H	-1.015644	-0.094094	-0.003623	0.3120	2.0000	1.320
H	0.326323	0.194580	-0.946601	0.3120	2.0000	1.320
H	1.271777	-1.698776	-0.300700	0.1000	2.7870	1.320
C	1.425506	-0.926083	1.755750	-0.0070	3.3080	2.040
C	1.261235	0.586898	1.991336	0.0189	3.3080	2.040
C	0.358899	1.122716	0.864265	-0.0120	3.3080	2.040
H	2.497463	-1.158459	1.585427	0.0253	2.8870	1.320
H	1.010291	-1.481414	2.622529	0.0253	2.8870	1.320
H	2.254535	1.078984	1.933818	0.0213	2.8870	1.320
H	0.767362	0.756029	2.970919	0.0213	2.8870	1.320
H	0.916608	1.879125	0.273583	0.1000	2.5000	1.320
H	-0.562245	1.557977	1.304881	0.1000	2.5000	1.320
O	-0.229185	-3.473245	0.426033	-0.7697	3.0612	1.824

Glutamine (Q), charge = 0						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	0.000000	-0.000000	0.000000	0.1493	3.2750	1.860
C	0.644349	-0.917009	-0.996950	0.0769	3.3080	2.040
C	1.976967	-1.427030	-0.502880	0.7775	3.3080	2.040
O	2.748700	-0.590320	0.013692	-0.8042	3.0612	1.824
H	-0.986378	-0.241115	0.096552	0.1996	2.0000	1.320
H	0.058078	0.961738	-0.334796	0.1996	2.0000	1.320
H	0.444436	-0.120280	0.910170	0.1996	2.0000	1.320
H	-0.012875	-1.794147	-1.172412	0.1015	2.7870	1.320
C	0.890270	-0.154964	-2.312400	-0.0036	3.3080	2.040
C	1.551801	-1.096427	-3.335935	-0.0645	3.3080	2.040
C	1.774946	-0.312652	-4.607156	0.6951	3.3080	2.040
O	2.287215	-0.804538	-5.599140	-0.6086	3.0612	1.824
N	1.551037	0.999340	-4.451795	-0.9407	3.2240	1.860
H	1.560482	0.708378	-2.118604	0.0171	2.8870	1.320
H	-0.078663	0.206100	-2.716012	0.0171	2.8870	1.320
H	0.860320	-1.933158	-3.567954	0.0352	2.8870	1.320
H	2.543560	-1.417367	-2.954475	0.0352	2.8870	1.320
H	1.263146	1.346954	-3.537091	0.4251	2.0000	1.320
H	1.428779	1.581643	-5.280274	0.4251	2.0000	1.320
O	2.206886	-2.647093	-0.648089	-0.8042	3.0612	1.824

Serine (S), charge = 0						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	-0.000000	0.000000	0.000000	0.1849	3.2750	1.860
C	-1.059165	-0.701041	-0.797943	0.0684	3.3080	2.040
C	-1.853894	-1.660646	0.055088	0.8113	3.3080	2.040
O	-1.208605	-2.398599	0.830670	-0.8132	3.0612	1.824
H	-0.005061	0.994430	-0.226897	0.1898	2.0000	1.320
H	0.916026	-0.374882	-0.246496	0.1898	2.0000	1.320
H	-0.202883	-0.097338	0.994869	0.1898	2.0000	1.320
H	-1.763948	0.047408	-1.216519	0.0782	2.7870	1.320
C	-0.398797	-1.512023	-1.928351	0.2117	3.3080	2.040
O	-1.428494	-2.151254	-2.648911	-0.6546	3.1210	1.824
H	0.228430	-2.315063	-1.488107	0.0352	2.7870	1.320
H	0.102275	-0.818489	-2.635483	0.0352	2.7870	1.320
H	-1.016566	-2.643197	-3.335866	0.4275	1.4001	1.320
O	-3.096535	-1.643971	-0.079321	-0.8132	3.0612	1.824

Threonine (T), charge = 0						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	0.000000	0.000000	-0.000000	0.1812	3.2750	1.860
C	0.342977	-0.746356	1.255117	0.0332	3.3080	2.040
C	-0.545093	-1.952791	1.444709	0.7810	3.3080	2.040
O	-1.769252	-1.792715	1.248975	-0.8044	3.0612	1.824
H	0.856916	0.238863	-0.499038	0.1934	2.0000	1.320
H	-0.477481	0.868753	0.240169	0.1934	2.0000	1.320
H	-0.562828	-0.595646	-0.607315	0.1934	2.0000	1.320
H	1.393294	-1.101168	1.199934	0.1087	2.7870	1.320
C	0.199840	0.192887	2.467113	0.3654	3.3080	2.040
O	0.530878	-0.548769	3.619701	-0.6761	3.1210	1.824
C	-1.268328	0.637671	2.602217	-0.2438	3.3080	2.040
H	0.945594	1.011367	2.389382	0.0043	2.7870	1.320
H	0.440801	0.031826	4.353456	0.4102	1.4001	1.320
H	-1.380972	1.315508	3.473967	0.0642	2.8870	1.320
H	-1.921616	-0.248069	2.746370	0.0642	2.8870	1.320
H	-1.588781	1.173188	1.684268	0.0642	2.8870	1.320
O	0.011555	-3.019673	1.782949	-0.8044	3.0612	1.824

Valine (V), charge = 0						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	0.000000	0.000000	-0.000000	0.0577	3.2750	1.860
C	0.922210	-1.182696	0.027563	0.0023	3.3080	2.040
C	0.720147	-2.073282	-1.174987	0.8350	3.3080	2.040
O	-0.459325	-2.336680	-1.494310	-0.8173	3.0612	1.824
H	0.521097	0.843721	0.238733	0.2272	2.0000	1.320
H	-0.734432	-0.124606	0.696767	0.2272	2.0000	1.320
H	-0.375460	0.117132	-0.941122	0.2272	2.0000	1.320
H	1.975231	-0.831732	0.019098	0.1093	2.7870	1.320
C	0.643280	-2.022803	1.287729	0.2985	3.3080	2.040
C	1.590082	-3.237038	1.316027	-0.3192	3.3080	2.040
C	0.875613	-1.160423	2.542289	-0.3192	3.3080	2.040
H	-0.408871	-2.376018	1.269939	-0.0297	2.8870	1.320
H	1.387647	-3.841322	2.224850	0.0791	2.8870	1.320
H	2.642210	-2.883814	1.334929	0.0791	2.8870	1.320
H	1.418162	-3.859745	0.413376	0.0791	2.8870	1.320
H	0.674132	-1.767479	3.449476	0.0791	2.8870	1.320
H	0.189360	-0.288207	2.522404	0.0791	2.8870	1.320
H	1.928867	-0.810467	2.559262	0.0791	2.8870	1.320
O	1.747740	-2.479284	-1.759550	-0.8173	3.0612	1.824

Tryptophan (W), charge = 0						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	0.000000	0.000000	0.000000	0.1913	3.2750	1.860
C	0.139846	-0.945450	1.156100	0.0555	3.3080	2.040
C	0.289602	-2.374152	0.690823	0.7658	3.3080	2.040
O	-0.484350	-2.761308	-0.211180	-0.8011	3.0612	1.824
H	0.596087	0.813700	0.151568	0.1888	2.0000	1.320
H	-0.965473	0.323426	-0.060483	0.1888	2.0000	1.320
H	0.307848	-0.461157	-0.856134	0.1888	2.0000	1.320
H	1.043948	-0.681377	1.743438	0.1162	2.7870	1.320
C	-1.095583	-0.828625	2.068059	-0.0050	3.3080	2.040
C	-0.955738	-1.774075	3.224159	-0.1415	3.3080	2.040
C	-0.381555	-1.493873	4.413403	-0.1638	3.3080	2.040
C	-1.381961	-3.054576	3.258084	0.1243	3.3080	2.040
N	-0.452915	-2.601199	5.182321	-0.3418	3.2240	1.860
C	-1.071200	-3.565767	4.468295	0.1380	3.3080	2.040
C	-2.012903	-3.821152	2.343331	-0.2387	3.3080	2.040
C	-1.391381	-4.843534	4.763753	-0.2601	3.3080	2.040
C	-2.333084	-5.098919	2.638789	-0.1972	3.3080	2.040
C	-2.022323	-5.610111	3.849001	-0.1134	3.3080	2.040
H	-2.006902	-1.086383	1.489129	0.0339	2.8870	1.320
H	-1.175430	0.210769	2.449352	0.0339	2.8870	1.320
H	0.065884	-0.532146	4.704739	0.2062	2.8090	1.320
H	-0.091060	-2.695651	6.163463	0.3412	2.0000	1.320
H	-2.266117	-3.404626	1.357234	0.1700	2.8590	1.320
H	-1.138168	-5.260060	5.749852	0.1572	2.8590	1.320
H	-2.847186	-5.723537	1.893434	0.1447	2.8590	1.320
H	-2.283210	-6.651253	4.089744	0.1417	2.8590	1.320
O	1.176117	-3.060866	1.243105	-0.8011	3.0612	1.824

Tyrosine (Y), charge = 0						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	-0.000000	0.000000	0.000000	0.1940	3.2750	1.860
C	-0.628053	0.944572	-0.981495	0.0766	3.3080	2.040
C	-2.039359	0.531922	-1.325058	0.7817	3.3080	2.040
O	-2.233716	-0.679076	-1.566327	-0.8070	3.0612	1.824
H	0.477767	0.532462	0.727064	0.1873	2.0000	1.320
H	0.694236	-0.575020	-0.477272	0.1873	2.0000	1.320
H	-0.726331	-0.560583	0.445634	0.1873	2.0000	1.320
H	-0.667809	1.963122	-0.542091	0.0983	2.7870	1.320
C	0.191259	0.950759	-2.285447	-0.0152	3.3080	2.040
C	-0.436794	1.895331	-3.266942	-0.0011	3.3080	2.040
C	-0.050248	3.230272	-3.291724	-0.1906	3.3080	2.040
C	-1.405335	1.435693	-4.151680	-0.1906	3.3080	2.040
C	-0.632244	4.105576	-4.201243	-0.2341	3.3080	2.040
C	-1.987331	2.310996	-5.061199	-0.2341	3.3080	2.040
C	-1.600786	3.645938	-5.085980	0.3226	3.3080	2.040
O	-2.170221	4.502350	-5.975869	-0.5579	3.1210	1.824
H	0.206508	-0.072155	-2.716161	0.0295	2.8870	1.320
H	1.228349	1.281099	-2.067687	0.0295	2.8870	1.320
H	0.716223	3.594014	-2.591572	0.1699	2.8590	1.320
H	-1.711235	0.379264	-4.132069	0.1699	2.8590	1.320
H	-0.326345	5.162004	-4.220854	0.1656	2.8590	1.320
H	-2.753803	1.947254	-5.761351	0.1656	2.8590	1.320
H	-2.814967	4.003457	-6.501520	0.3992	1.4001	1.320
O	-2.905796	1.432754	-1.342024	-0.8070	3.0612	1.824

Histidine (H), charge = +1						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	0.000000	0.000000	-0.000000	0.2560	3.2750	1.860
C	1.452136	-0.295884	-0.231846	0.0653	3.3080	2.040
C	1.742404	-0.544670	-1.692651	0.8032	3.3080	2.040
O	0.951365	-1.290578	-2.309400	-0.8177	3.0612	1.824
H	-0.088670	0.797647	0.629521	0.1704	2.0000	1.320
H	-0.444411	-0.803300	0.444532	0.1704	2.0000	1.320
H	-0.442844	0.246341	-0.885215	0.1704	2.0000	1.320
H	2.063648	0.571028	0.094677	0.1047	2.7870	1.320
C	1.862975	-1.530775	0.591474	-0.0414	3.3080	2.040
C	3.315111	-1.826659	0.359628	-0.0012	3.3080	2.040
N	4.349090	-1.335743	1.075441	-0.1513	3.2240	1.860
C	3.817512	-2.630624	-0.601482	-0.1141	3.3080	2.040
C	5.490525	-1.836305	0.556728	-0.0170	3.3080	2.040
N	5.161992	-2.636586	-0.479667	-0.1718	3.2240	1.860
H	1.253933	-2.403507	0.276026	0.0810	2.8870	1.320
H	1.695745	-1.327287	1.669772	0.0810	2.8870	1.320
H	4.280026	-0.698505	1.868888	0.3866	2.0000	1.320
H	3.233848	-3.183740	-1.352082	0.2317	2.8090	1.320
H	6.509394	-1.628563	0.915546	0.2681	2.7590	1.320
H	5.814954	-3.154770	-1.067481	0.3911	2.0000	1.320
O	2.751619	0.014241	-2.173902	-0.8177	3.0612	1.824

Lysine (K), charge = +1						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	0.000000	-0.000000	0.000000	0.0966	3.2750	1.860
C	-0.474967	1.397043	0.269587	-0.0101	3.3080	2.040
C	-1.874782	1.408725	0.835696	0.8488	3.3080	2.040
O	-2.716296	0.667209	0.283872	-0.8252	3.0612	1.824
H	0.954757	-0.107087	0.342595	0.2165	2.0000	1.320
H	0.005121	-0.169753	-1.005763	0.2165	2.0000	1.320
H	-0.590991	-0.663228	0.501257	0.2165	2.0000	1.320
H	0.196412	1.880307	1.009727	0.1180	2.7870	1.320
C	-0.492624	2.196910	-1.046279	-0.0094	3.3080	2.040
C	-0.980257	3.631207	-0.769503	0.0187	3.3080	2.040
C	-0.997914	4.431073	-2.085369	-0.0479	3.3080	2.040
C	-1.485547	5.865370	-1.808593	-0.0143	3.3080	2.040
N	-1.502745	6.644460	-3.090281	-0.3854	3.2750	1.860
H	-1.179962	1.706382	-1.766729	0.0362	2.8870	1.320
H	0.532512	2.231436	-1.470547	0.0362	2.8870	1.320
H	-0.292918	4.121734	-0.049053	0.0103	2.8870	1.320
H	-2.005393	3.596680	-0.345234	0.0103	2.8870	1.320
H	-1.685253	3.940545	-2.805820	0.0621	2.8870	1.320
H	0.027222	4.465599	-2.509638	0.0621	2.8870	1.320
H	-0.790820	6.360383	-1.098370	0.1135	2.5000	1.320
H	-2.515742	5.831513	-1.396705	0.1135	2.5000	1.320
H	-1.825723	7.594449	-2.906962	0.3400	2.0000	1.320
H	-2.131647	6.193262	-3.754587	0.3400	2.0000	1.320
H	-0.561897	6.674555	-3.483090	0.3400	2.0000	1.320
O	-2.085427	2.159021	1.813032	-0.8252	3.0612	1.824

Arginine (R), charge = +1						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	0.000000	0.000000	0.000000	0.1305	3.2750	1.860
C	0.026755	-1.484164	-0.215733	-0.0359	3.3080	2.040
C	0.080723	-1.831533	-1.684243	0.8557	3.3080	2.040
O	-0.689992	-1.206066	-2.444040	-0.8266	3.0612	1.824
H	0.652030	0.247689	0.744249	0.2083	2.0000	1.320
H	-0.934825	0.284786	0.292233	0.2083	2.0000	1.320
H	0.299892	0.473404	-0.852264	0.2083	2.0000	1.320
H	0.928240	-1.912943	0.269627	0.1242	2.7870	1.320
C	-1.251795	-2.111876	0.369834	-0.0007	3.3080	2.040
C	-1.224326	-3.635618	0.148349	0.0390	3.3080	2.040
C	-2.502877	-4.263330	0.733915	0.0486	3.3080	2.040
N	-2.477013	-5.698022	0.525373	-0.5295	3.2240	1.860
C	-3.502068	-6.461796	0.959437	0.8076	3.3080	2.040
N	-3.477988	-7.797544	0.765278	-0.8627	3.2240	1.860
N	-4.551202	-5.889823	1.587661	-0.8627	3.2240	1.860
H	-2.139895	-1.681410	-0.138179	0.0327	2.8870	1.320
H	-1.302401	-1.898316	1.457920	0.0327	2.8870	1.320
H	-0.336226	-4.066084	0.656362	0.0285	2.8870	1.320
H	-1.173719	-3.849178	-0.939738	0.0285	2.8870	1.320
H	-3.390977	-3.832863	0.225902	0.0687	2.7870	1.320
H	-2.553483	-4.049769	1.822002	0.0687	2.7870	1.320
H	-1.684334	-6.130179	0.050715	0.3456	2.0000	1.320
H	-4.252473	-8.374618	1.093237	0.4478	2.0000	1.320
H	-2.685309	-8.229702	0.290620	0.4478	2.0000	1.320
H	-5.325687	-6.466897	1.915620	0.4478	2.0000	1.320
H	-4.569395	-4.880592	1.734359	0.4478	2.0000	1.320
O	0.892002	-2.718096	-2.028238	-0.8266	3.0612	1.824

Glutamate (E), charge = −1						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	0.000000	0.000000	-0.000000	0.0017	3.2750	1.860
C	-1.481201	0.180683	-0.152959	0.0698	3.3080	2.040
C	-2.187361	-1.142390	-0.328783	0.7420	3.3080	2.040
O	-1.674598	-1.957870	-1.125380	-0.7930	3.0612	1.824
H	0.336779	0.582913	0.766284	0.2391	2.0000	1.320
H	0.469632	0.300126	-0.854266	0.2391	2.0000	1.320
H	0.202267	-0.972596	0.231400	0.2391	2.0000	1.320
H	-1.890904	0.667877	0.756374	0.1202	2.7870	1.320
C	-1.768523	1.037066	-1.400218	0.0560	3.3080	2.040
C	-3.289222	1.222567	-1.557256	0.0136	3.3080	2.040
C	-3.526855	2.064994	-2.787682	0.8054	3.3080	2.040
O	-4.714983	2.323000	-3.078003	-0.8188	3.0612	1.824
O	-2.517342	2.440190	-3.422199	-0.8188	3.0612	1.824
H	-1.364613	0.526338	-2.299170	-0.0173	2.8870	1.320
H	-1.285935	2.029992	-1.284868	-0.0173	2.8870	1.320
H	-3.685244	1.778148	-0.681702	-0.0425	2.8870	1.320
H	-3.766038	0.234043	-1.723290	-0.0425	2.8870	1.320
O	-3.230903	-1.321386	0.335657	-0.7930	3.0612	1.824

Aspartate (D), charge = −1						
Atom	x	y	z	q_{AMBER}	R_{AMBER}	R_{HF}
N	0.000000	0.000000	0.000000	0.0782	3.2750	1.860
C	-1.256901	-0.534658	0.619952	0.0326	3.3080	2.040
C	-1.528279	0.100684	1.962633	0.7256	3.3080	2.040
O	-0.560798	0.204377	2.747317	-0.7887	3.0612	1.824
H	-0.167756	0.208258	-0.984320	0.2200	2.0000	1.320
H	0.732936	-0.707459	0.052029	0.2200	2.0000	1.320
H	0.266414	0.867949	0.464855	0.2200	2.0000	1.320
H	-2.119739	-0.313969	-0.042550	0.1141	2.7870	1.320
C	-1.117462	-2.052882	0.837105	-0.0303	3.3080	2.040
C	-2.399780	-2.549672	1.460770	0.7994	3.3080	2.040
O	-2.472115	-3.771942	1.712410	-0.8014	3.0612	1.824
O	-3.291287	-1.700809	1.677903	-0.8014	3.0612	1.824
H	-0.291824	-2.248685	1.552706	-0.0122	2.8870	1.320
H	-0.998273	-2.556383	-0.144923	-0.0122	2.8870	1.320
O	-2.699739	0.474540	2.187164	-0.7887	3.0612	1.824

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