## Exploration of the Conformational and Reactive Dynamics of Biomolecules in Solution using an Extended Version of the Glycine Reactive Force Field

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## **Force Field Parametrization and Validation**

Zijing Lin and co-workers: Amino Acids. The amino acid structures added to the trainset were obtained through systematic quantum mechanical studies carried out at the DFT-B3LYP/6-311++G\*\* level of theory. The authors conducted exhaustive conformational searches building all combinations of internal single-bond rotamers and performed energy optimization of the generated conformations without any constraint. Subsequent checks, comprising harmonic frequencies and single point calculations at a higher level of theory (MP2/6-311G(2df,p)//B3LYP/6-311++G\*\*), allowed for the identification of the lowest energy conformers. [TRAINSET]

Kaminsky and Jensen: Dipeptides. Kaminsky and Jensen sampled and optimized, at the DFT and MP2 levels with an augmented double-zeta basis set, the conformational degrees of freedom of glycine, alanine, serine and cysteine. They obtained the best estimate of the relative conformational energies by means of an extrapolation procedure of the MP2 energy results (extrapolation to the basis set limit and CCSD(T) correction - see Reference for details) and used these data as reference to check the performance of eight different force fields. The comparison revealed that only half of the conformations were identified by the force fields based on fixed partial charges, whereas those including multipoles and polarizability, could reproduce most of the structures. These structures, which comprised two Gly, seven Ala, thirty-eight Ser and forty-seven Cys conformations, were not included in ReaxFF training set but were used as test case to check the parameters and assess the validity of the new reactive force field. [VALIDATION]

**Hobza and co-workers: Oligopeptides.** Hobza and co-workers performed theoretical studies on the performance of different levels of theory in comparison with the CCSD(T)/CBS benchmark for Phe-Gly-Phe (FGF), Trp-Gly (WG), Trp-Gly-Gly (WGG), Phe-Gly-Gly (FGG), Gly-Gly-Phe (GGF) and Gly-Phe-Ala (GFA) peptides. On the basis of experimental observations they restricted the benchmark study to fifteen different conformers for each species, which were selected following a procedure defined in earlier investigations [Valdés, H.; Pluhackova, K.; Hobza, P. J. Chem. Theory Comput. 2009, 5, 2248]. Geometry optimizations were performed at the RI-MP2/cc-pVTZ level of theory and also by means of the AMBER ff99 force field with the HF/6-31G\* RESP charges. In their conclusion the authors did not recommend the use of this force field for investigations in the gas phase but suggested that a reliable strategy could be to use three different levels of theory, namely tight-binding DFT-D, RI-MP2 or M06-2X, and MP2/CBS for the study of the potential energy surface of the peptide, the reoptimization of selected structures and single-point energy calculations, respectively.

Some of these structures (fifteen WG, fifteen WGG and sixteen GFA conformations), were included in ReaxFF training set, whereas the others (fifteen FGF, fifteen FGG and fifteen GGF conformations) were used as test case to validate the developed parameters. [TRAINSET]+[VALIDATION]

Martin Head-Gordon and co-workers : Tetrapeptides, Octapeptides and Hexadecapeptides. A series of polypeptide conformations, made of alanine residues, were employed by Martin Head-Gordon and co-workers [Di Stasio, R. A.; Jung, Y.; Head-Gordon, M. J. Chem. Theory Comput. 2005, 1, 862] to appraise the overall performance of the RI-TRIM MP2 method against other techniques in the prediction of the relative energies of the structures. The main sample consisted of twenty seven different geometries of the alanine tetrapeptide, but octapeptide, and hexadecapeptide structures were also present among

the deposited data. All the conformations were optimized at the HF/6-31G\*\* level and in addition, they also performed single-point energy calculations with higher levels and with different basis sets. The authors concluded that the accurate prediction of the relative energies of the series of tetrapeptides implies calculations with the cc-pVTZ and cc-pVQZ basis sets and then extrapolation to the cc-pV(TQ)Z limit. This data was not part of training set, but it was used for validation. **[VALIDATION]** 

## **Protein Models and Structured Oligopeptides**

**Crambin.** Crambin is a small protein consisting of 46 amino acids, it has been used as test case for a wide variety of simulations mainly for two reasons **1**) its crystal and solution structures have been resolved to a high degree of accuracy (0.48 Å) in the best case [*Schmidt, A.; Teeter, M.; Weckert, E.; Lamzin, V. S. Acta Cryst. 2011, F67, 424*]) **2**) it contains different secondary structure elements (two antiparallel  $\alpha$ -helices, a short segment of anti parallel  $\beta$ -sheet and a classical  $\beta$ -turn), hydrophilic and hydrophobic residues, a salt bridge (between Arg10 and the terminal Asn46 carboxyl) and three disulfide bridges that are expected to reduce the overall conformational freedom of the molecule.

The protein is quite hydrophobic and, even though it is small, it presents well defined charged areas. There are two negative regions around the C-terminus and the  $\beta$ -turn, while the preponderant flat surface is positively charged. The protein does not contain reactive residues or a definite active site, thus its role is accomplished by its structure, shape and surface properties.

**Tryptophan Cage.** TRP-cage is a synthetic miniprotein made of 20 amino acids with a cooperatively folded tertiary structure, a globular shape and a combination of secondary structure motifs and tertiary contacts typical of more complex proteins [*Neidigh, J. W.; Fesinmeyer, R. M.; Andersen, N. H. Nat. Struct. Biol. 2002, 9, 425; Gellman, S. H.; Woolfson, D. N. Nat. Struct. Biol. 2002, 9, 408*]. It was designed by Neidigh and co-workers [*Neidigh, J. W.; Fesinmeyer, R. M.; Andersen, N. H. Nat. Struct. Biol. 2002, 9, 425*] to explore the folding pathways and understand the stability of globular proteins from both an experimental and theoretical point of view. Indeed, this protein is an ideal choice because it is able to fold quickly (in about 4  $\mu$ s) and spontaneously to a native state where a short  $\alpha$ -helix (residues 2-9), a 3<sub>10</sub> helix (residues 11-14) and a polyproline II helix at the C-terminus are present. All these secondary structure elements are packed against the central tryptophan residue (TRP6) [*Neidigh, J. W.; Fesinmeyer, R. M.; Andersen, N. H. Nat. Struct. Biol. 2002, 9, 425; Qiu, L.; Pabit, S. A.; Roitberg, A. E. J. Am. Chem. Soc. 2002, 124, 12952*] and shield it from the solvent action.

TRP-cage has been well characterized from an experimental point of view and many simulations have been carried out using both implicit and explicit solvent models to disclose the different folding events. However, it was observed that, as in many other cases, solvent effects play a crucial role in conformational dynamics and molecular stability and thus a more realistic representation of the systems should be obtained if explicit solvent molecules are added as a surrounding medium. These models differ from a continuum solvent description as they take into account local effect and specific perturbations to the macromolecular structures.

**Oligopeptides.** The selected short structured oligopeptides are the C-terminal  $\beta$ -hairpin of G protein [Blanco, F. J.; Rivas, G.; Serrano, L. Nat. Struct. Biol. 1994, 1, 584] (**protG**), the synthetic EK  $\alpha_R$ -helix [Scholtz, J. M.; Barrick, D.; York, E. J.; Stewart, J. M.; Baldwin, R. L. Proc. Natl. Acad. Sci.U.S.A. 1995, 92, 185] (**EK**), the helical C peptide of ribonuclease A [Bierzynski, A.; Kim, P. S.; Baldwin, R. L. Proc. Natl. Acad. Sci. U.S.A. 1982, 79, 2470] (**Baldwin**) and the synthetic trpzip2 hairpin [Cochran, A. G.; Skelton, N. J.; Starovasnik, M. A. Proc. Natl. Acad. Sci. U.S.A. 2001, 98, 5578] (**trpzip2**).

Briefly, **protG** has a  $\beta$ -hairpin conformation which is stabilized by four salt bridges, and hydrophobic interactions between the Tyr/Phe and Trp/Val residue pairs. The polar nature of **EK**, which contains two AEAAKA segments, confers to the molecule an  $\alpha$ -helical conformation; **Baldwin** is a 13-amino acid helix partially stabilized by a salt bridge and **trpzip2** consists of 12 residues arranged as a hairpin due to the interactions between the side chains of its Trp residues (stacking complexes) and a salt bridge between Glu5 and Lys8 charged side chains.

Reactive MD-force field: prot\_ff + GFA WGG WG Hobza\_DB. March20 2012 ! Number of general parameters 39 50.0000 !Overcoordination parameter 9.5469 !Overcoordination parameter 1.6725 !Valency angle conjugation parameter 1.7224 !Triple bond stabilisation parameter 6.8702 !Triple bond stabilisation parameter 60.4850 !C2-correction 1.0588 !Undercoordination parameter 4.6000 !Triple bond stabilisation parameter 12.1176 !Undercoordination parameter 13.3056 !Undercoordination parameter -40.0000 !Triple bond stabilization energy 0.0000 !Lower Taper-radius 10.0000 !Upper Taper-radius 2.8793 !Not used 33.8667 !Valency undercoordination 6.0891 !Valency angle/lone pair parameter 1.0563 !Valency angle 2.0384 !Valency angle parameter 6.1431 !Not used 6.9290 !Double bond/angle parameter 0.3989 !Double bond/angle parameter: overcoord 3.9954 !Double bond/angle parameter: overcoord -2.4837 !Not used 5.7796 !Torsion/BO parameter 10.0000 !Torsion overcoordination 1.9487 !Torsion overcoordination -1.2327 !Conjugation 0 (not used) 2.1645 !Conjugation 1.5591 !vdWaals shielding 0.1000 !Cutoff for bond order (\*100) 1.7602 !Valency angle conjugation parameter 0.6991 !Overcoordination parameter 50.0000 !Overcoordination parameter 1.8512 !Valency/lone pair parameter 0.5000 !Not used 20.0000 !Not used 5.0000 !Molecular energy (not used) 0.0000 !Molecular energy (not used) 0.7903 !Valency angle conjugation parameter 11 ! Nr of atoms; cov.r; valency; a.m; Rvdw; Evdw; gammaEEM; cov.r2; # alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u. cov r3;Elp;Heat inc.;n.u.;n.u.;n.u.;n.u. ov/un;val1;n.u.;val3,vval4 1.3817 4.0000 12.0000 1.8903 С 0.1838 0.6387 1.1341 4.0000 9.7559 2.1346 4.0000 34.9350 79.5548 4.9218 6.0000 0.0000 0.0000 202.2908 8.9539 34.9289 13.5366 2.5000 1.0564 4.0000 2.9663 0.0000 1.2114 0.8563 0.0000 0.0000 0.0000 -2.8983 0.0000 н 0.8930 1.0000 1.0080 1.3550 0.0930 0.8203 -0.1000 1.0000 1.0000 3.7248 9.6093 0.0000 121.1250 1.0000 8.2230 33.2894 0.0000 55.1878 -0.1000 3.0408 2.4197 0.0003 1.0698 0.0000 4.2733 1.0338 1.0000 2.8793 0.0000 0.0000 -19.4571 0.0000 1.2450 2.0000 15.9990 2.3890 0.1000 1.0898 1.0548 6.0000 0 9.7300 13.8449 4.0000 37.5000 116.0768 8.5000 8.3122 2.0000 0.4056 68.0152 0.9049 3.5027 0.7640 0.0021 0.9745 0.0000 -3.5500 2.9000 1.0493 4.0000 2.9225 0.0000 0.0000 0.0000 3.0000 14.0000 2.1294 0.1322 1.0000 1.1748 N 1.2333 5.0000 6.4603 10.0056 10.8657 4.0000 30.9146 100.0000 2.0000 7.0317 4.7941 119.9837 0.6005 7.9731 2.2800 0.9745 1.0433 0.0000 -4.6366 4.0000 1.0183 4.0000 2.8793 0.0000 0.0000 0.0000 S 1.9673 2.0000 32.0600 2.1729 0.3000 1.0336 1.5359 6.0000 4.0000 52.9998 112.1416 10.3008 4.9055 6.5000 8.2545 2.0000 9.7177 71.1843 5.7487 23.2859 12.7147 1.4601 0.9745 0.0000 0.0000 -11.0000 2.7466 1.0338 6.2998 2.8793 0.0000 0.0000 2.0000 24.3050 1.8315 2.2464 0.1806 0.5020 1.0000 2.0000 Mq 10.9186 27.1205 3.0000 38.0000 0.0000 0.9499 5.6130 0.0000 -1.3000 0.0000 220.0000 49.9248 0.3370 0.0000 0.0000 0.0000 -1.0823 2.3663 1.0564 6.0000 2.9663 0.0000 0.0000 0.0000

| 9.1909         14.2932         5.0000         0.0000         1.2822         7.2520         0.0000           -2.5000         1.6114         1.3338         5.0000         2.4733         0.0000         0.0000         1.000           1.0000         9.8000         1.0000         0.0000         0.0000         1.000         1.000         1.000           -1.0000         0.0000         1.0200         0.0000 <td< th=""><th>Ρ</th><th>1</th><th>L.5994</th><th>3.0000 30</th><th>0.9738</th><th>1.7000</th><th>0.1743</th><th>1.000</th><th>0 1.</th><th>3000</th><th>5.0000</th></td<>   | Ρ  | 1   | L.5994    | 3.0000 30              | 0.9738     | 1.7000                                  | 0.1743            | 1.000             | 0 1.    | 3000    | 5.0000  |
|---|----|-----|-----------|------------------------|------------|---|-------------------|-------------------|---------|---------|---------|
| <ul> <li>-1.0000 10.2596 1.5000 0.2205 16.7429 15.9629 0.000 0.000</li> <li>-2.5000 1.6114 1.0338 5.0000 2.3793 0.0000 0.0505 1.0948 0.000</li> <li>-0.000 0.0000 0.0000 0.0000 0.0000 0.2550 0.9456 0.000</li> <li>-0.000 0.0000 0.1338 6.0000 2.5791 0.0000 0.0000 0.000</li> <li>-2.5766 2.5000 1.0338 6.0000 2.791 0.0000 0.0000 0.000</li> <li>-1.9202 2.0000 63.5460 1.9221 0.2826 1.0000 0.000 0.000</li> <li>-1.9202 2.0000 63.5460 1.9221 0.2826 1.0000 0.000 0.0563 0.000</li> <li>-1.9202 2.0000 63.5460 1.9221 0.2826 1.0000 0.000 0.000</li> <li>-1.9202 3.0000 80.7000 34.9555 0.4988 0.0000 0.3837 -1.0000 7.00</li> <li>-1.000 0.0000 80.7000 34.9555 0.4988 0.0000 0.3837 -1.0000 7.00</li> <li>-1.000 3.5750 143.1770 6.2293 5.2294 0.1542 0.8563 0.00</li> <li>-1.000 3.5750 143.1770 6.2293 5.2294 0.1542 0.8563 0.00</li> <li>-1.000 3.5750 143.1770 6.2293 5.2294 0.1542 0.8563 0.00</li> <li>-0.0998 2.0000 1.0080 2.0000 0.0000 1.0000 -0.1000 0.000</li> <li>-0.0098 2.9867 1.0338 6.2998 2.2994 0.1500 0.0000 0.000</li> <li>-0.0000 0.25000 -2.3700 8.7410 13.840 0.0000 1.0000 -0.1000 6.000</li> <li>-0.1000 0.25000 -2.3700 8.7410 13.840 0.0000 1.0000 -0.0000 0.000</li> <li>-0.1000 0.0000 -0.7738 -0.4550 1.0000 37.6117 0</li> <li>-0.4590 -0.1000 9.1628 1.0000 -0.0777 6.7268 1.0000 1</li> <li>1.153476 0.0000 0.0000 -0.0033 0.0000 1.0000 6.0552 0.0000 0</li> <li>-5.2290 1.0000 0.0000 -0.0033 0.0000 1.0000 6.0552 0.0000 0</li> <li>-5.2394 0.0000 0.0000 -0.0333 6.9316 0.0000 0</li> <li>-5.2394 0.0000 0.0000 -0.0333 6.9316 0.0000 0</li> <li>-5.2394 0.0000 0.0000 -0.0333 6.9316 0.0000 0</li> <li>-5.2394 0.0000 0.0000 -0.0334 0.0000 1.0000 8.5623 0.1000 0</li> <li>-5.2393 0.2566 -0.1000 1.0000 8.5623 0.1000 0</li> <li>-5.2394 0.0000 0.0000 -0.0334 0.0000 1.0000 8.563 0.1000 0</li> <li>-5.2394 0.0000 0.0000 -0.0334 0.0000 1.0000 8.5617 0</li> <li>-5.2394 0.0000 0.0000 -0.0335 5.0000 1.0000 8.5617 0</li> <li>-5.2394 0.0000 0.0000</li></ul>  |    | 9   | 9.1909 14 | 4.2932 !               | 5.0000     | 0.0000                                  | 0.0000            | 1.829             | 27.     | 2520    | 0.0000  |
| -2.5000         1.6114         1.0338         5.0000         2.7933         0.0000         0.0000         1.000           11.0000         9.8000         1.0000         0.0000         0.0000         1.0000         0.00000         0.00000 </td <td></td> <td>-1</td> <td>L.0000 1</td> <td>0.2596</td> <td>1.5000</td> <td>0.2205</td> <td>16.7429</td> <td>15.962</td> <td>90.</td> <td>0000</td> <td>0.0000</td>   |    | -1  | L.0000 1  | 0.2596                 | 1.5000     | 0.2205                                  | 16.7429           | 15.962            | 90.     | 0000    | 0.0000  |
| Na         2.0300         1.0000         22.9898         2.3344         0.1481         0.8765         -1.0000         1.0000         0.0000         0.3000         0.0000         0.3563         0.000           -1.0000         0.0000         67.5458         100.0000         1.0000         0.0556         0.000           -1.9202         2.0000         63.5460         1.9221         0.2826         1.0000         0.1000         0.0000           -1.9000         0.0000         2.5791         0.0000         0.0000         0.0000         0.0000         0.0000           -1.0000         0.0000         3.550         1.9498         0.0000   |    | -2  | 2.5000    | 1.6114 1               | 1.0338     | 5.0000                                  | 2.8793            | 0.000             | 0 0.    | 0000    | 0.0000  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   | Na | 2   | 2.0300    | 1.0000 22              | 2.9898     | 2.3334                                  | 0.1481            | 0.876             | 5 -1.   | 0000    | 1.0000  |
| $\begin{array}{c} -1.0000 & 0.0000 & 67.5458 & 100.0000 & 10.0000 & 0.2570 & 0.25803 & 0.000 & 0.000 & 0.000 & 0.0000 & 0.$  |    | 11  | L.0000    | 9.8000                 | 1.0000     | 0.0000                                  | 0.0000            | -3.850            | 1 5.    | 9459    | 0.0000  |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  |    | -1  | L.0000    | 0.0000 6'              | 7.5458 10  | 0.0000                                  | 10.0000           | 0.250             | 00.     | 8563    | 0.0000  |
| Cu 1.9202 2.0000 63.5460 1.9221 0.2826 1.0000 0.1000 1.000<br>-1.0000 0.0000 1.0000 0.0000 2.7875 6.0000 0.0000<br>-5.1872 3.1491 1.0000 34.9555 0.4988 0.0000 0.8563 0.00<br>-1.0000 3.5750 143.1700 6.2293 5.2294 0.1542 0.8563 0.00<br>-1.02000 3.5750 143.1700 6.2293 5.2294 0.1542 0.8563 0.00<br>-1.02000 2.9867 1.0338 6.2998 2.5791 0.0000 0.0000 0.000<br>10.0000 2.9867 1.0338 6.2998 2.5791 0.0000 0.0000 0.000<br>-0.1000 0.0000 -2.3700 8.7410 13.8640 0.6690 0.9745 0.00<br>-0.1000 0.0000 -2.3700 8.7410 13.8640 0.6690 0.9745 0.00<br>-1.10000 2.7466 1.0338 4.0000 2.8793 0.0000 1.0000 -0.000<br>-1.0000 0.0000 -0.7300 8.7410 13.8640 0.6690 0.9745 0.00<br>-1.10000 2.7466 1.0338 4.0000 -0.7773 6.7268 1.0000 0<br>0.4590 -0.1000 9.1628 1.0000 -0.7776 6.7268 1.0000 0<br>5.2290 1.0000 0.0000 -0.6683 0.0000 1.0000 6.0000 0<br>5.2290 1.0000 0.0000 -0.6683 0.0000 1.0000 6.0000 0<br>0.5220 1.0000 0.0000 -0.6683 0.0000 1.0000 6.0000 0<br>0.6.5200 1.0000 0.0000 -0.6683 0.0000 1.0000 6.0000 0<br>0.52290 1.0000 0.0000 -0.6683 0.0000 1.0000 6.0000 0<br>0.4510 -0.1554 9.0144 8.9489 1.0000 -0.5554 6.2210 0.0000 0<br>0.3 3142.2858 145.000 5.8293 0.2506 -0.1000 1.0000 0.5550 0.0000 0<br>1 4.164.1304 141.330 102.0444 -1.8021 -0.5546 1.0000 2.7639 0<br>0.3531 -0.3663 7.1330 1.0000 -0.1225 5.5000 1.0000 0<br>1 4.164.1304 141.330 102.0444 -1.8021 -0.5546 1.0000 2.7639 0<br>0.33142.2858 167.8643 40.0000 0.3819 -0.1539 1.0000 34.9972 0<br>1.0110 -0.3716 7.8653 1.0000 -0.2575 0.0000 1.0000 0<br>2 4.211.6032 0.0000 0.0000 1.0000 -0.2559 0.0000 0<br>2 4.214.032 0.0000 0.0000 -0.5552 0.0000 0<br>1 4.164.1304 141.336 102.0444 -1.8021 -0.5546 1.0000 2.7639 0<br>0.0331 -0.257 1.5559 1.0000 0.0000 -0.2575 0.0000 1.0000 0<br>2 4.216.032 5.7712 7.554 1.0000 -0.7753 5.4371 1.0000 0<br>2 4.217.0335 5.2526 153.9844 0.4110 -0.9344 1.0000 1.0000 0<br>0 1.5138 -0.1473 11.9187 1.0000 -0.753 5.4371 1.0000 0<br>1 4.164.1304 140.335 5.228 -0.6281 1.0000 1.0000 0<br>1 4.2429 -0.4771 12.759 1.0000 -0.0753 5.4371 1.0000 0<br>0 .0327 -0.3315 5.2520 153.9846 0.4111 -0.9434 1.0000 1.89647 0<br>0 .0326 -0.5133 9.127 1.0000 -0.0754 5.6673   |    | -2  | 2.5766    | 2.5000                 | 1.0338     | 6.0000                                  | 2.5791            | 0.000             | 0 0.    | 0000    | 0.0000  |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | Cu | 1   | L.9202    | 2.0000 63              | 3.5460     | 1.9221                                  | 0.2826            | 5 1.000           | 0 0.    | 1000    | 1.0000  |
| <ul> <li>-1.000 0.000 80.7000 34.9555 0.4988 0.0000 0.8853 0.00</li> <li>-5.1872 3.1491 1.0000 4.0000 2.5791 0.0000 0.0000 7.00</li> <li>11.5345 10.1330 1.0000 0.0000 0.0000 9.9614 6.5316 0.00</li> <li>-10.000 3.5750 143.1770 6.2293 5.2294 0.1542 0.8563 0.00</li> <li>-10.000 2.9667 1.0338 6.2998 2.5791 0.0000 0.0000 0.000</li> <li>-0.0098 2.0000 1.0080 2.0000 0.0000 1.0000 -0.1000 6.00</li> <li>-0.0000 2.5000 4.0000 0.0000 0.0000 1.0000 -0.1000 6.00</li> <li>-0.1000 2.5000 4.0000 0.0000 0.0000 1.0000 -0.1000 6.00</li> <li>-0.1000 2.5000 4.0000 0.0000 0.85000 1.5000 0.00</li> <li>-0.1000 2.7466 1.0338 4.0000 2.8793 0.0000 0.0000 37.6117 0</li> <li>10.58.2004 9.1897 78.0000 -0.773 -0.4550 1.0000 37.6117 0</li> <li>0.4590 -0.1000 9.1628 1.0000 -0.0777 6.7268 1.0000 0</li> <li>2.169.4760 0.0000 0.0000 1.0000 -0.0553 6.9316 0.0000 0</li> <li>2.5290 1.0000 0.0000 1.0000 -0.0553 6.9316 0.0000 0</li> <li>2.5201 1.0000 0.0000 1.0000 -0.0770 6.5552 0.0000 0</li> <li>2.5201 1.0000 0.0000 1.0000 -0.0790 6.5552 0.0000 0</li> <li>2.513.3934 0.0000 0.0000 1.0000 -0.1225 5.5000 1.0000 0</li> <li>3.142.2858 145.0000 50.8293 0.2566 -0.1000 1.0000 2.8753 0</li> <li>0.3451 -0.1555 9.0001 0.0001 -0.1225 5.500 1.0000 0</li> <li>0.3451 -0.0559 0.0001 0.001 -0.1255 4.6940 1.0000 2.0000 0</li> <li>4.164.1304 141.330 102.0464 -1.8021 -0.5594 1.0000 34.9972 0</li> <li>1.6110 -0.376 7.8051 1.0000 -0.1255 6.8843 1.0000 0</li> <li>4.128.856 167.6643 40.0000 0.3189 -0.1539 1.0000 34.9972 0</li> <li>0.3314 -0.2475 1.528 15.3884 0.4110 -0.0934 1.0000 12.4304 0</li> <li>0.1538 -0.1473 11.9187 1.0000 -0.1255 6.8843 1.0000 0</li> <li>4.164.1304 141.3360 102.0464 -1.8021 -0.1539 1.0000 34.9972 0</li> <li>0.1513 -0.1473 11.9187 1.0000 -0.1255 6.8843 1.0000 0</li> <li>2.1633 2.92552 15.3884 0.4110 -0.0934 1.0000 12.4304 0</li> <li>0.3317 -0.2289 1.5282 0.0000 0.0000 -0.1418 1.0000 12.4304 0</li> <li>0.3314 -0.2494 9.8465 1.0000 -0.</li></ul>  |    | 1(  | 0.9889 10 | 0.0000                 | 1.0000     | 0.0000                                  | 0.0000            | 2.787             | 56.     | 0000    | 0.0000  |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  |    | -1  | L.0000    | 0.0000 80              | 0.7000 3   | 4.9555                                  | 0.4988            | 3 0.000           | 00.     | 8563    | 0.0000  |
| C1 1.7140 1.0000 35.4500 1.9139 0.2000 0.9814 6.5316 0.00<br>-1.02080 2.9867 1.0338 6.2998 2.5791 0.0000 0.0000 0.000<br>-0.0008 2.9867 1.0338 6.2998 2.5791 0.0000 0.0000 0.000<br>-0.0000 2.5000 4.0000 0.0000 0.0000 1.0000 -0.1000 6.00<br>-0.1000 0.5000 4.0000 0.0000 0.0000 1.0000 0.0000<br>-0.1000 0.0000 -2.3700 8.7410 13.3640 0.6690 0.9745 0.00<br>-0.1000 2.7466 1.0338 4.0000 2.8793 0.0000 0.0000 37.6117 0<br>-0.1000 2.7466 1.0338 4.0000 2.8793 0.0000 0.0000 37.6117 0<br>-0.4590 -0.1000 9.1628 1.0000 -0.0777 6.7268 1.0000 0<br>0.4590 -0.1000 9.1628 1.0000 -0.0777 6.7268 1.0000 0<br>1 2 169.4760 0.0000 0.0000 -0.0683 0.0000 1.0000 6.0000 0<br>5.2290 1.0000 0.0000 -0.0683 0.0000 1.0000 6.0000 0<br>6.2500 1.0000 0.0000 -0.0683 0.0000 1.0000 6.0000 0<br>6.2500 1.0000 0.0000 -0.4600 0.0000 1.0000 6.0000 0<br>3 3 142.2858 145.0000 50.8293 0.2566 -0.1000 18.9948 0<br>1.5618 -0.3414 8.949 1.0000 -0.1255 5.5000 1.0000 0<br>3 3 142.2858 145.0000 50.8293 0.2566 -0.1000 18.9948 0<br>1.5618 -0.3714 8.949 1.0000 -0.1255 5.5000 1.0000 0<br>3 3 142.2858 145.0000 50.8293 0.2566 -0.1000 12.76095 0<br>0.3553 -0.3663 7.1330 1.0000 -0.2557 4.6940 1.0000 0<br>3 4 128.596 157.8643 40.000 0.3819 -0.1539 1.0000 27.6095 0<br>0.3553 -0.3663 7.1330 1.0000 -0.2557 4.6940 1.0000 0<br>3 4 128.596 157.8643 40.000 0.3819 -0.1539 1.0000 34.9972 0<br>1.0110 -0.3716 7.0805 1.0000 -0.1255 5.4371 1.0000 12.4304 0<br>0.1538 -0.1473 11.9187 1.0000 -0.0753 5.4371 1.0000 0<br>2 4 211.6322 0.0000 0.0000 -0.5725 0.0000 1.0000 6.0000 0<br>2 5 143.4377 0.0000 0.0000 -0.5744 1.0000 18.9617 0<br>0.3317 -0.2289 7.5946 1.0000 -0.1165 5.6864 1.0000 0<br>2 5 143.4377 0.0000 0.0000 -0.0753 5.4371 1.0000 0<br>2 5 143.4377 0.0000 0.0000 -0.0753 5.4371 1.0000 0<br>2 5 143.4377 0.0000 0.0000 -0.0753 5.4371 1.0000 0<br>2 5 143.4377 0.0000 0.0000 -0.0254 -0.438 1.0000 12.4304 0<br>0 0.3217 -0.1289 7.5946 1.0000 -0.1805 7.0960 1.0000 0<br>2 5 143.4377 0.0000 0.0000 -0.2554 -0.4038 1.0000 12.4304 0<br>0 0.3216 -0.3153 9.1227 1.0000 -0.188 1.0000 13.1260 0<br>0 0.3216 -0.3150 9.0000 1.0000 -0.1418 1.0000 13.1260 0<br>0 0.3216 -0.3150 0.0000  |    | - 5 | 5.1872    | 3.1491                 | 1.0000     | 4.0000                                  | 2.5791            | 0.000             | 0 0.    | 0000    | 0.0000  |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | C1 | ]   | L.7140    | 1.0000 3               | 5.4500     | 1.9139                                  | 0.2000            | 0.383             | 7 -1.   | 0000    | 7.0000  |
| <ul> <li>-10.000</li> <li>-10.2080</li> <li>2.9567</li> <li>1.0338</li> <li>6.2998</li> <li>2.5791</li> <li>0.0000</li> <li>0.0000<td></td><td>11</td><td>L.5345 1</td><td>0.1330</td><td>1.0000</td><td>0.0000</td><td>0.0000</td><td>9.961</td><td>46.</td><td>5316</td><td>0.0000</td></li></ul>   |    | 11  | L.5345 1  | 0.1330                 | 1.0000     | 0.0000                                  | 0.0000            | 9.961             | 46.     | 5316    | 0.0000  |
| <ul> <li>-10.2080 2.9867 1.0338 6.2998 2.5791 0.0000 0.0000 0.000 0.000</li> <li>-0.1000 1.0000 1.0000 0.0000 0.0000 0.0000 0.0000 0.000</li> <li>-0.1000 0.2.5000 4.0000 0.0000 0.0000 8.5000 1.5000 0.000</li> <li>-11.0000 2.7466 1.0338 4.0000 2.8793 0.0000 0.0000 0.000</li> <li>+ Nr of bonds; Edist, Lppen; n.u., pbe1; pb5; J320cr; pb0</li> <li>-11.858, 2004 99.1897 78.0000 -0.7738 -0.4550 1.0000 7776 5.7268 1.0000 0</li> <li>2.159.4760 0.0000 0.0000 -0.6683 0.0000 1.0000 6.0000 0</li> <li>2.159.4760 0.0000 0.0000 -0.6683 0.0000 1.0000 6.0000 0</li> <li>2.2153.3934 0.0000 0.0000 -0.4600 0.0000 1.0000 6.0000 0</li> <li>2.2153.3934 0.0000 0.0000 -0.4600 0.0000 1.0000 6.0552 0.0000 0</li> <li>3.115.3161 127.1552 61.7072 0.5141 -0.3744 1.0000 18.9948 0</li> <li>1.5618 -0.3414 8.9489 1.0000 -0.1628 5.6821 0.0000 0</li> <li>3.142.2858 145.0000 50.2939 0.2566 -0.1000 1.0000 29.7503 0</li> <li>0.3451 -0.1055 9.0000 1.0000 -0.1225 5.5000 1.0000 0</li> <li>4.164.1304 141.3380 102.0464 -1.8021 -0.5696 1.0000 29.7503 0</li> <li>0.3953 -0.3663 7.130 1.0000 -0.2557 4.6940 1.0000 0</li> <li>4.128.8556 167.8643 40.0000 0.3819 -0.1539 1.0000 12.4304 0</li> <li>0.1538 -0.1473 11.9187 1.0000 -0.2557 4.6940 1.0000 0</li> <li>4.160.1592 82.5526 153.9884 0.4110 -0.0934 1.0000 12.4304 0</li> <li>0.1518 -0.1473 11.9187 1.0000 -0.0753 5.4371 1.0000 0</li> <li>4.160.1592 82.5528 153.9884 0.4110 -0.0924 4.2790 0.0000 0</li> <li>1.1150 1.0000 0.0000 -0.0725 0.0001 1.0000 6.0000 0</li> <li>2.1180 1.0000 0.0000 -0.0244 0.0000 1.0000 6.0000 0</li> <li>2.1317 -0.2289 7.5964 1.0000 -0.1946 5.9455 1.0000 0</li> <li>2.1483 4377 0.0000 0.0000 -0.2744 1.0000 1.0000 6.0000 0</li> <li>2.1488 1.0000 0.0000 -0.2744 0.0000 1.0000 6.0000 0</li> <li>2.1488 4.9350 6.6660 -0.4111 -0.4781 1.0000 40.3399 0</li> <li>0.3266 -0.3153 9.1227 1.0000 -0.1866 5.6332 1.0000 0</li> <li>4.2250 -0.4259 1.2494 9.8436 1.0000 -0.2695 6.4254 0.0000 2</li></ul>   |    | -1  | L.0000    | 3.5750 14              | 3.1770     | 6.2293                                  | 5.2294            | 0.154             | 20.     | 8563    | 0.0000  |
| <pre>x -0.0998 2.0000 1.0000 0.0000 0.0000 1.0000 -0.1000 0.00</pre>  |    | -1( | 0.2080    | 2.9867                 | 1.0338     | 6.2998                                  | 2.5791            | 0.000             | 0 0.    | 0000    | 0.0000  |
| 10.0000         2.5000         +.0000         0.0000         0.5000         1.5000         0.000         0.000         0.000           -11.0000         2.7466         1.0338         4.0000         2.8793         0.0000         0.000         0.000           43         1 Nr of bonds: Edial:LEpeninipbel;pbo5;l3corr         pbe2;pbo3;pbo4;Etrip;pbo1;pbo2;ovcorr           1         158.204         99.1897         78.0000         -0.7738         -0.4550         1.0000         7.66117           0         0.4590         -0.1000         9.1628         1.0000         -0.0777         6.7268         1.0000         0           1         158.2001         1.0000         -0.0000         1.0000         -0.0553         6.9316         0.0000         0           3         115.3161         127.1552         61.772         0.5141         -0.3744         1.0000         1.8948         0           1.5618         -0.3414         8.9489         1.0000         -0.1225         5.5000         1.0000         0           3         142.8586         143.360         10.200         -0.1255         4.6940         1.0000         0           3         142.3845         167.8643         40.0000         0.3819  | Х  | -(  | 0.0998    | 2.0000 .               | 1.0080     | 2.0000                                  | 0.0000            | 1.000             | 0 -0.   | 1000    | 6.0000  |
| -10.1000 0.0000 -2.3700 8.7410 13.3640 0.6890 0.9745 0.000<br>-11.0000 2.7466 1.0338 4.0000 2.8793 0.0000 0.0000 0.000<br>43 ! Nr of bonds: Edis1LiPpenrin.u.;bpel;bb5;l3corr;bb6<br>pb2;bb3;bb6;lEtri;pb6);b0;vocorr<br>1 1 158.2004 99.1897 78.0000 -0.7738 -0.4550 1.0000 37.6117 0<br>0.4590 -0.1000 9.1628 1.0000 -0.0777 6.7268 1.0000 0<br>5.2290 1.0000 0.0000 -0.6083 0.0000 1.0000 6.0000 0<br>6.2500 1.0000 0.0000 -0.6083 0.0000 1.0000 6.0000 0<br>0.52290 1.0000 0.0000 -0.4600 0.0000 1.0000 6.0000 0<br>1 3 115.3161 127.1562 61.7072 0.5141 -0.3474 1.0000 18.9948 0<br>1.5618 -0.3414 8.9489 1.0000 -0.0258 5.600 1.0000 27.6095 0<br>0.3451 -0.1055 9.0000 1.0000 -0.2557 4.6540 0.0000 0<br>3 142.2858 145.0000 50.8293 0.2506 -0.1000 1.0000 27.6095 0<br>0.3451 -0.1055 9.0000 1.0000 -0.2557 4.6540 1.0000 0<br>4 164.1304 141.3380 102.0464 -1.8021 -0.5696 1.0000 27.6095 0<br>0.3935 -0.3663 7.1330 1.0000 -0.1255 5.000 1.0000 44.9972 0<br>1.0110 -0.3716 7.0805 1.0000 -0.0254 4.6540 1.0000 0<br>4 160.1592 82.5526 153.9884 0.4110 -0.0374 1.0000 12.4304 0<br>0.1538 -0.1473 11.9187 1.0000 -0.0753 5.4371 1.0000 0<br>2 3 160.0000 0.0000 0.0000 -0.5725 0.0000 1.0000 1.0000 6<br>2 4 211.6032 0.0000 0.0000 -0.3415 0.0000 1.0000 12.4304 0<br>0.1538 -0.1473 11.9187 1.0000 -0.0753 5.4371 1.0000 10<br>2 3 160.0000 0.0000 0.0000 -0.3714 5.6399 0.00000 0<br>2 4 211.6032 0.0000 0.0000 -0.3415 0.0000 1.0000 6.0000 0<br>2 5 143.4377 0.0000 0.0000 -0.3415 0.0000 1.0000 6.0000 0<br>5 5 140.887 84.9356 68.660 -0.4111 -0.4781 1.0000 18.9617 0<br>0.3277 1.0000 0.0000 1.0000 -0.1145 5.9455 1.0000 0<br>5 5 140.887 84.9356 68.660 -0.4111 -0.4781 1.0000 18.9617 0<br>0.4259 -0.4577 12.7569 1.0000 -0.1005 5.6464 1.0000 0<br>6 5 140.887 84.9350 68.660 -0.4111 -0.4781 1.0000 13.2260 0<br>3 5 0.0000 0.0000 0.0000 -0.223 -0.1418 1.0000 49.5611 0<br>0.02864 1-0.2300 10.0000 1.0000 -0.2645 5.9455 1.0000 0<br>2 7 0.1466 0.0000 0.0000 0.2500 -0.4398 6.673 1.0000 4<br>4 6 32.3808 0.0000 0.0000 -0.203 -0.1418 1.0000 13.1260 0<br>0.3601 -0.1310 10.7257 1.0000 -0.869 5.3302 1.0000 0<br>0.03912 -0.1310 0.0000 1.0000 -0.2085 6.53302 1.0000  |    | ΤC  | 10000     | 2.5000                 | 4.0000     | 0.0000                                  | 12 2640           | 8.500             | U I.    | 5000    | 0.0000  |
| 11.000         2.7466         1.0338         4.0000         2.8793         0.0000         0.0000         0.000           1         158.2004         99.1897         78.0000         -0.7738         -0.4550         1.0000         0           1         158.2004         99.1628         1.0000         -0.0777         6.7268         1.0000         0           1         2.169.4760         0.0000         0.0000         -0.0000         0.0000         1.0000         6.0552         0.0000         0           2         2.153.3934         0.0000         0.0000         -0.0790         6.0552         0.0000         0           3         3.142.2858         145.0000         5.08293         0.2566         -0.1000         1.0000         29.7503         0           0.3451         -0.1555         9.0000         1.0000         -0.2557         4.6940         1.0000         0           1.0101         -0.3716         7.0851         1.0000         -0.1255         5.5000         1.0000         0           1.1110         -0.3716         7.0851         1.0000         -0.2557         4.6940         1.0000         0         1.4164.1304         1414.13380         1.0000         -0.2557   |    | -(  | 0.1000    | 0.0000 - 2             | 2.3/00     | 8.7410                                  | 13.3640           | 0.669             | 0 0.    | 9/45    | 0.0000  |
| <ul> <li>A. F. R. D. DORGS, EditS L. DEPER, FLO. T. DEET, PDOS (1980) 1980</li></ul>  | 12 | -11 |           | 2./400 .<br>E bendat 1 | L.U338     | 4.0000                                  | 2.8/93            | 5 U.UUU           | 0 0.    | 0000    | 0.0000  |
| DBC2/DB3/DB3/DB3/DB3/DE17D1/DB02/DB02/DB03/DB17           1         158.2004         99.1897         78.0000         -0.4550         1.0000         7.0417         0.04550           1         2163.4760         0.0000         0.0000         -0.6583         0.0000         1.0000         6.0200         0           2         153.3934         0.0000         0.0000         -0.6553         6.9316         0.0000         0           2         153.3934         0.0000         0.0001         -0.0790         6.0552         0.0000         0           3         115.3161         127.1562         61.7072         0.5141         -0.3474         1.0000         29.7503         0           3         3         142.2858         145.000         0.8293         0.2506         -0.1000         1.0000         27.6595         0           0.3451         -0.1055         9.0000         1.0000         -0.2557         4.6940         1.0000         0           1         14164.1304         141.3380         10.20464         -1.8021         -0.5696         1.0000         1.0000         1.0000         1.0000         1.0000         1.0000         1.0000         1.0000         1.0000         1.0000         1.0000  | 43 |     | INF O     |                        | Laisi, LPP | 2. mbo 4.                               | , poer, pr        | 005,13COL         | r, ppoe |         |         |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   | 1  | 1   | 159 2004  | 00 1007                |            | -0.77                                   | so _0 V           | 1550 1            | 0000rr  | 27 6117 | 0 4147  |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | T  | T   | 156.2004  | -0 1000                | 0 1620     |   | 00 -0.4           | 1550 $1.$         | 7269    | 1 0000  | 0.4147  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   | 1  | 2   | 169 4760  | -0.1000                | 9.1020     |   |                   | 1000 1            | 0000    | £ 0000  | 0.0000  |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | T  | 2   | 5 2200    | 1 0000                 | 0.0000     | 1 0.00                                  |                   | )000 I.           | 0000    | 0.0000  | 0.7052  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   | 2  | 2   | 153 3034  | 0.0000                 | 0.0000     | -0.46                                   |                   | 1000 1            | 0000    | 6 0000  | 0.0000  |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | 2  | 2   | 6 2500    | 1 0000                 | 0.0000     | 1 0.40                                  | 00 -0.0           | 1790 E            | 0552    | 0.0000  | 0.7500  |
| $ \begin{array}{c} 1.5618 & -0.3414 \\ 1.5618 & -0.3414 \\ 1.000 & 50.8293 \\ 0.2506 & -0.1000 \\ 1.0000 & 29.7503 \\ 0.3451 & -0.1055 \\ 9.0000 \\ 1.0000 & -0.1225 \\ 5.5000 \\ 1.0000 & 27.6095 \\ 0 \\ 0.3953 & -0.3663 \\ 7.1330 \\ 1.0000 & -0.2557 \\ 4.6940 \\ 1.0000 \\ 27.6095 \\ 0 \\ 1.0110 & -0.3716 \\ 7.0805 \\ 1.0000 \\ -0.355 \\ 1.0000 \\ 1.0110 \\ -0.3716 \\ 7.0805 \\ 1.0000 \\ -0.355 \\ 1.0000 \\ 1.0100 \\ 0.315 \\ 1.0000 \\ 0.0000 \\ 1.0100 \\ 0.0153 \\ 1.0000 \\ 0.0000 \\ 1.0$ | 1  | З   | 115 3161  | 127 1562               | 61 7072    | 0 51                                    | 41 -0 3           | 8474 1            | 0000    | 18 9948 | 0.0000  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   | -  | 5   | 1.5618    | -0.3414                | 8.9489     | 1.00                                    | 00 -0.1           | 628 5.            | 6821    | 0.0000  | 0.0000  |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | 3  | 3   | 142,2858  | 145.0000               | 50.8293    | 0.25                                    | 06 -0.1           | 000 1.            | 0000    | 29.7503 | 0.6051  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   | 5  | 5   | 0.3451    | -0.1055                | 9.0000     | 1.00                                    | 00 -0.1           | 225 5.            | 5000    | 1.0000  | 0.0000  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   | 1  | 4   | 164.1304  | 141.3380               | 102.0464   | -1.80                                   | 21 -0.5           | 5696 1.           | 0000    | 27.6095 | 0.2487  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   |    |     | 0.3953    | -0.3663                | 7.1330     | 1.00                                    | 00 -0.2           | 2557 4.           | 6940    | 1.0000  | 0.0000  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   | 3  | 4   | 128.8596  | 167.8643               | 40.0000    | 0.38                                    | 19 -0.1           | .539 1.           | 0000    | 34.9972 | 0.1900  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   |    |     | 1.0110    | -0.3716                | 7.0805     | 1.00                                    | 00 -0.1           | 265 6.            | 8843    | 1.0000  | 0.0000  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   | 4  | 4   | 160.1592  | 82.5526                | 153.9884   | 0.41                                    | 10 -0.0           | 934 1.            | 0000    | 12.4304 | 0.5899  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   |    |     | 0.1538    | -0.1473                | 11.9187    | 1.00                                    | 00 -0.0           | )753 5.           | 4371    | 1.0000  | 0.0000  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   | 2  | 3   | 160.0000  | 0.0000                 | 0.0000     | -0.57                                   | 25 0.0            | 0000 1.           | 0000    | 6.0000  | 0.5626  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   |    |     | 1.1150    | 1.0000                 | 0.0000     | 0.00                                    | 00 -0.0           | 920 4.            | 2790    | 0.0000  | 0.0000  |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | 2  | 4   | 211.6032  | 0.0000                 | 0.0000     | -0.34                                   | 15 0.0            | 0000 1.           | 0000    | 6.0000  | 0.4726  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   |    |     | 2.7198    | 1.0000                 | 0.0000     | 1.00                                    | 00 -0.1           | .744 5.           | 6399    | 0.0000  | 0.0000  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   | 1  | 5   | 150.8132  | 59.3363                | 55.2528    | -0.06                                   | 28 -0.5           | 5211 1.           | 0000    | 18.9617 | 0.3219  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   |    |     | 0.3317    | -0.2289                | 7.5946     | 1.00                                    | 00 -0.1           | .946 5.           | 9455    | 1.0000  | 0.0000  |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | 2  | 5   | 143.4377  | 0.0000                 | 0.0000     | -0.29                                   | 44 0.0            | 0000 1.           | 0000    | 6.0000  | 0.6034  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   |    |     | 9.5627    | 1.0000                 | 0.0000     | 1.00                                    | 00 -0.0           | )516 7.           | 0960    | 1.0000  | 0.0000  |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | 3  | 5   | 0.0000    | 0.0000                 | 0.0000     | 0.55                                    | 63 -0.4           | 1.                | 0000    | 49.5611 | 0.6000  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   |    |     | 0.4259    | -0.4577                | 12.7569    | 1.00                                    | 00 -0.1           | 100 7.            | 1145    | 1.0000  | 0.0000  |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | 4  | 5   | 0.0000    | 0.0000                 | 0.0000     | 0.44                                    | 38 -0.2           | 2034 1.           | 0000    | 40.3399 | 0.6000  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   | -  | -   | 0.3296    | -0.3153                | 9.1227     | 1.00                                    | 00 -0.1           | 805 5.            | 6864    | 1.0000  | 0.0000  |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | 5  | 5   | 140.888/  | 84.9350                | 68.6860    | -0.41                                   | 11 -0.4           | E/81 I.           | 4720    | 1 0000  | -0.1336 |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | 2  | c   | 0.2881    | -0.2494                | 9.8436     |   |                   | 410 1             | 4/32    | 12 12CO | 0.0000  |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | 2  | 0   | 58.6896   | 0.0000                 | 0.0000     | 1 -0.02                                 | 03 -0.1           | .418 1.           | 4054    | 13.1200 | 0.0230  |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | 2  | c   | 8.2136    | -0.1310                | 42 2001    | 1.00                                    |                   | 2692 6.           | 4254    | 0.0000  | 24.4461 |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   | 3  | 0   | 87.0227   | 0.0000                 | 43.3991    | . 0.00                                  | 30 -0.3           | 3000 I.           | 0000    | 1 0000  | 0.0250  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   | c  | c   | 0.008/    | -0.2500                | 12.0000    |   | 00 -0.0<br>76 0 0 | 1439 6.           | 0000    | 16 0000 | 24.4461 |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$  | 0  | 0   | 32.3000   | 0.0000                 | 10.0000    |   | 70 -0.2           | 2000 0.           | C 2 1 0 | 10.0000 | 0.2041  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   | 1  | 7   | 4.8/20    | -0.2000                | 10.0000    |   | 00 -0.0<br>71 0 1 | 1/29 4.<br>110 1  | 0000    | 12 1260 | 0.0000  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   | T  | /   | 0 2601    | 92.0000                | 10 7255    | 1 0.21                                  | /1 -0.1           | 1410 I.           | 2202    | 1 0000  | 0.0000  |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   | 2  | 7   | 0.3001    | -0.1310                | 0 0000     | 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 | 50 -0.U           | 418 <sup>1</sup>  | 0000    | 13 1060 | 0.0000  |
| 3         7         202.5868         164.1808         0.0000         0.5506         -0.1029         9.3302         0.0000         0           3         7         202.5868         164.1808         0.0000         0.5506         -0.5000         1.0000         25.0000         0           0.0912         -0.1285         16.0342         1.0000         -0.2008         6.2678         1.0000         0           4         7         130.0000         0.0000         0.2171         -0.1418         1.0000         13.1260         0           0.3601         -0.1310         10.7257         1.0000         -0.0869         5.3302         1.0000         0           6         7         0.1000         0.0000         0.2500         -0.5000         1.0000         35.0000         0           0.5000         -0.5000         20.0000         1.0000         -0.2000         10.0000         0  | 4  | /   | 0.1400    | _0 1310                | 0.0000     | 1 1 00                                  | 00 _0.1           | . 120 1.<br>120 0 | 2202    | 0 0000  | 0.0000  |
| 0.0912       -0.1285       16.0342       1.0000       -0.2008       6.2678       1.0000       0         4       7       130.0000       0.0000       0.2171       -0.1418       1.0000       13.1260       0         0.3601       -0.1310       10.7257       1.0000       -0.0869       5.3302       1.0000       0         6       7       0.1000       0.0000       0.2500       -0.5000       1.0000       35.0000       0         6       7       0.1000       0.0000       1.0000       -0.2000       10.0000       1.0000       0   | 2  | 7   | 202 5860  | 164 1909               | 0.0000     | ) 1.00                                  | 06 _0.1           | 5000 1            | 0000    | 25 0000 | 0.0000  |
| 4         7         130.0000         0.0000         0.2171         -0.1418         1.0000         13.1260         0           0.3601         -0.1310         10.7257         1.0000         -0.0869         5.3302         1.0000         0           6         7         0.1000         0.0000         0.2500         -0.5000         1.0000         0           0.55000         -0.5000         20.0000         1.0000         -0.2000         10.0000         0  | د  | /   | 0 0010    | -0 1285                | 16 02/2    | 0.55                                    | 00 _0.5           | 2000 I.           | 2678    | 1 0000  | 0.4300  |
| 0.3601         -0.1310         10.7257         1.0000         -0.0869         5.3302         1.0000         0           6         7         0.1000         0.0000         0.2500         -0.5000         1.0000         0           0.5000         -0.5000         20.0000         1.0000         -0.2000         10.0000         0   | 4  | 7   | 130 0000  | 0 0000                 | 0 00012    | ) <u>1.00</u>                           | 71 _0.1           | 418 1             | 0000    | 13,1260 | 0 6000  |
| 6 7 0.1000 0.0000 0.0000 0.2500 -0.5000 1.0000 35.0000 0<br>0.5000 -0.5000 20.0000 1.0000 -0.2000 10.0000 0   | -  | ,   | 0.3601    | -0.1310                | 10,7257    | 1 00                                    | 00 -0.0           | )869 5            | 3302    | 1.0000  | 0.0000  |
| 0.5000 -0.5000 20.0000 1.0000 -0.2000 10.0000 1.0000 0  | б  | 7   | 0.1000    | 0.0000                 | 0,0000     | 0.25                                    | 00 -0.5           | 5000 1            | 0000    | 35.0000 | 0,6000  |
|   | 0  |     | 0.5000    | -0.5000                | 20.0000    | 1.00                                    | 00 -0.2           | 2000 10.          | 0000    | 1.0000  | 0.0000  |
| 7 7 0.0000 0.0000 0.0000 0.2171 -0.5000 1.0000 35.0000 0  | 7  | 7   | 0.0000    | 0.0000                 | 0.0000     | 0.21                                    | 71 -0.5           | 5000 1.           | 0000    | 35.0000 | 0.6000  |

|     |    | 0.5000    | -0.5000     | 20.0000  | 1.0000   | 0 -0.2000  | 10.0000   | 1.0000   | 0.0000 |
|-----|----|-----------|-------------|----------|----------|------------|-----------|----------|--------|
| 2   | 8  | 0.0000    | 0.0000      | 0.0000   | -1.0000  | 0 -0.3000  | 1.0000    | 36.0000  | 0.7000 |
|     |    | 10.1151   | -0.3500     | 25.0000  | 1.0000   | 0 -0.1053  | 8.2003    | 1.0000   | 0.0000 |
| 3   | 8  | 76.0753   | 0.0000      | 0.0000   | -0.4452  | 2 -0.3000  | 1.0000    | 36.0000  | 0.6433 |
|     |    | 5.6834    | -0.3500     | 25.0000  | 1.0000   | 0 -0.0539  | 8.0273    | 1.0000   | 0.0000 |
| 4   | 8  | 0.0000    | 0.0000      | 0.0000   | -1.0000  | 0.3000     | 1.0000    | 36.0000  | 0.7000 |
|     |    | 10.1151   | -0.3500     | 25.0000  | 1.0000   | 0 -0.1053  | 8.2003    | 1.0000   | 0.0000 |
| б   | 8  | 0.1000    | 0.0000      | 0.0000   | 0.2500   | 0 -0.5000  | 1.0000    | 35.0000  | 0.6000 |
|     |    | 0.5000    | -0.5000     | 20.0000  | 1.0000   | 0 -0.2000  | 10.0000   | 1.0000   | 0.0000 |
| 7   | 8  | 0.1000    | 0.0000      | 0.0000   | 0.2500   | 0 -0.5000  | 1.0000    | 35.0000  | 0.6000 |
|     |    | 0.5000    | -0.5000     | 20.0000  | 1.0000   | 0 -0.2000  | 10.0000   | 1.0000   | 0.0000 |
| 8   | 8  | 27.8052   | 0.0000      | 0.0000   | 0.4022   | 2 0.3000   | 0.0000    | 25.0000  | 0.4894 |
|     |    | 0.6222    | -0.4000     | 12.0000  | 1.0000   | 0 -0.0500  | 5.3362    | 0.0000   | 0.0000 |
| 4   | 6  | 0.0000    | 0.0000      | 0.0000   | -1.0000  | 0 -0.3000  | 1.0000    | 36.0000  | 0.7000 |
| _   | _  | 10.1151   | -0.3500     | 25.0000  | 1.0000   | ) -0.1053  | 8.2003    | 1.0000   | 0.0000 |
| 1   | 9  | 0.0000    | 0.0000      | 0.0000   | 0.2000   | 0 -0.1418  | 1.0000    | 13.1260  | 0.5000 |
| _   | _  | 0.5000    | -0.2000     | 20.0000  | 1.0000   | ) -0.1000  | 9.0000    | 0.0000   | 0.0000 |
| 2   | 9  | 0.0000    | 0.0000      | 0.0000   | 0.2000   | ) -0.1418  | 1.0000    | 13.1260  | 0.5000 |
|     |    | 0.5000    | -0.2000     | 20.0000  | 1.0000   | ) -0.1000  | 9.0000    | 0.0000   | 0.0000 |
| 3   | 9  | 81.4346   | 0.0000      | 0.0000   | -0.1594  | 4 -0.3000  | 1.0000    | 36.0000  | 0.0025 |
|     |    | 0.2904    | -0.2500     | 12.0000  | 1.0000   | ) -0.0742  | 9.3638    | 0.0000   | 0.0000 |
| 4   | 9  | 96.5322   | 0.0000      | 0.0000   | 0.9970   | ) -0.3000  | 1.0000    | 36.0000  | 0.5095 |
| •   | ~  | 0.7247    | -0.2500     | 12.0000  | 1.0000   | ) -0.1175  | 9.9985    | 0.0000   | 0.0000 |
| 9   | 9  | 73.6263   | 0.0000      | 0.0000   | 0.0209   | 9 -0.2000  | 0.0000    | 16.0000  | 0.3414 |
| ~   | 10 | 0.4703    | -0.2000     | 15.0000  | 1.0000   | J -0.1319  | 5.9254    | 0.0000   | 0.0000 |
| 2   | ΤU | 109.1686  | 0.0000      | 0.0000   | -0.165   |            | 0.0000    | 16.0000  | 1.2500 |
| 2   | 10 | 2.8463    | -0.2000     | 15.0000  | 1.0000   |            | 5.2687    | 0.0000   | 0.0000 |
| 3   | ΤU | 1 0001    | 0.0000      | 15 0000  | 1 0000   | J = 0.2000 | 10.0000   | 16.0000  | 0.5000 |
| 0   | 10 | 110 20E2  | -0.2000     | 15.0000  | 0 116    | J -0.1000  | 10.0000   | 16 0000  | 0.0000 |
| 9   | ΤU | 2 0176    | -0.2000     | 15 0000  | -0.1100  | -0.2000    | 5 2624    | 10.0000  | 0.0097 |
| 10  | 10 | 2.9170    | -0.2000     | 13.0000  | 0 1901   | -0.1310    | 0 0000    | 16 0000  | 0.0000 |
| 10  | τu | 0.2500    | -0.2000     | 15 0000  | 1 0000   | -0.2000    | 5 6715    | 10.0000  | 0.3350 |
| 1   | Q  | 0.9228    | 0.2000      | 13.0000  | -1 0000  | 0.11/0     | 1 0000    | 36 0000  | 0.0000 |
| 1   | 0  | 10 1151   | -0.2500     | 25 0000  | 1 0000   | -0.3000    | 2 2002    | 1 0000   | 0.7000 |
| 1   | 10 | 0 0000    | 0.0000      | 23.0000  | 0 5000   | -0.1033    | 0 0000    | 16 0000  | 0.0000 |
| T   | τU | 1 0001    | -0 2000     | 15 0000  | 1 0000   | -0.2000    | 10 0000   | 0 0000   | 0.0000 |
| 4   | 10 | 0 0000    | 0.0000      | 0 0000   | 0 5000   |            | 10.0000   | 16 0000  | 0.0000 |
| 1   | τu | 1 0001    | -0 2000     | 15 0000  | 1 0000   | -0.1000    | 10 0000   | 0 0000   | 0.0000 |
| 22  |    | ! Nr of c | off-diagon; | al terms | ; Ediss; | Ro;gamma;r | sigma;rpi | rpi2     | 0.0000 |
| 1   | 2  | 0.1239    | 1.4004      | 9.8467   | 1.1210   | -1.0000    | -1.0000   |          |        |
| 2   | 3  | 0.0283    | 1.2885      | 10,9190  | 0.921    | 5 -1.0000  | -1.0000   |          |        |
| 2   | 4  | 0.1664    | 1.3100      | 9.6406   | 1.0569   | 9 -1.0000  | -1.0000   |          |        |
| 1   | 3  | 0.0503    | 1.8006      | 10.2114  | 1.3492   | 2 1.1992   | 1.0506    |          |        |
| 1   | 4  | 0.1771    | 1.8995      | 9.6891   | 1.3428   | 3 1.2492   | 1.1154    |          |        |
| 3   | 4  | 0.2000    | 1.8388      | 9.5137   | 1.458    | 7 1.0933   | 1.1826    |          |        |
| 1   | 5  | 0.1618    | 1.7943      | 10.1042  | 1.7489   | 9 1.3150   | 1.4031    |          |        |
| 2   | 5  | 0.0764    | 1.5838      | 10.1462  | 1.4200   | 5 -1.0000  | -1.0000   |          |        |
| 3   | 5  | 0.1022    | 1.9887      | 10.0605  | 1.5799   | 9 1.4000   | -1.0000   |          |        |
| 4   | 5  | 0.1505    | 1.9000      | 10.5104  | 1.8000   | 0 1.4000   | -1.0000   |          |        |
| 2   | б  | 0.0100    | 1.6000      | 13.2979  | 1.8670   | 0 -1.0000  | -1.0000   |          |        |
| 3   | б  | 0.0809    | 1.7000      | 11.4606  | 1.517    | 7 -1.0000  | -1.0000   |          |        |
| 3   | 7  | 0.0611    | 1.7624      | 10.2685  | 1.7989   | 9 1.4523   | -1.0000   |          |        |
| 6   | 7  | 0.1801    | 1.8566      | 9.8498   | 0.1000   | 0 -1.0000  | -1.0000   |          |        |
| 3   | 8  | 0.1592    | 1.8283      | 11.7256  | 1.665    | 5 -1.0000  | -1.0000   |          |        |
| 1   | 9  | 0.0500    | 1.7500      | 12.3500  | 0.1000   | 0 -1.0000  | -1.0000   |          |        |
| 2   | 9  | 0.0300    | 1.5200      | 12.5000  | 0.1000   | 0 -1.0000  | -1.0000   |          |        |
| 3   | 9  | 0.0348    | 1.7637      | 12.3562  | 1.7228   | 8 -1.0000  | -1.0000   |          |        |
| 4   | 9  | 0.0478    | 1.7704      | 12.8051  | 1.6100   | 0 -1.0000  | -1.0000   |          |        |
| 2   | 10 | 0.0568    | 1.6740      | 9.6297   | 1.2200   | 0 -1.0000  | -1.0000   |          |        |
| 3   | 10 | 0.1927    | 2.2551      | 11.2308  | -1.0000  | 0 -1.0000  | -1.0000   |          |        |
| 9   | 10 | 0.1402    | 2.1604      | 10.9786  | 1.750    | 5 -1.0000  | -1.0000   |          |        |
| 104 |    | ! Nr of a | ingles;at1  | ;at2;at3 | ;Thetao, | ;ka;kb;pv  | 1;pv2     |          |        |
| 1   | 1  | 1 59.05   | 30.70       | 29 0.7   | 506 0.0  | 0.00 0.7   | 180 6.2   | 933 1.12 | 244    |
| 1   | 1  | 2 65.77   | 58 14.52    | 34 6.24  | 481 0.0  | 0.5        | 665 0.0   | 000 1.62 | 255    |
| 2   | 1  | 2 70.26   | 07 25.22    | 02 3.7   | 312 0.0  | 0.0 0000   | 050 0.0   | 000 2.7  | 500    |
| 1   | 2  | 2 0.00    | 0.00        | 00 6.0   | 0.0      | 0.0 0000   | 000 0.0   | 000 1.04 | 100    |
| 1   | 2  | 1 0.00    | 3.41        | 10 7.7   | 350 0.0  | 0.0 0000   | 000 0.0   | 000 1.04 | 100    |
| 2   | 2  | 2 0.00    | 00 27.92    | 13 5.8   | 635 0.0  | 0.0 0000   | 000 0.0   | 000 1.04 | 400    |

| 1      | 1      | 3                   | 54.7427            | 21.1992            | 1.0613           | 0.0000   | 2.9950           | 58.6562 | 1.1232 |
|--------|--------|---------------------|--------------------|--------------------|------------------|----------|------------------|---------|--------|
| 3      | 1      | 3                   | 78.6632            | 16.3065            | 6.3613           | -19.9300 | 1.5183           | 0.0000  | 2.2234 |
| 1      | 1      | 4                   | 78.9895            | 29.7448            | 1.4146           | 0.0000   | 1.1834           | 0.0000  | 2.4298 |
| 3      | 1      | 4                   | 74.5431            | 30.9283            | 1.2618           | 0.0000   | 1.1019           | 0.0000  | 1.0888 |
| 4      | 1      | 4                   | 90.0000            | 15.9388            | 0.5081           | 0.0000   | 1.1155           | 0.0000  | 2.5891 |
| 2      | 1      | 3                   | 50.0000            | 12.9103            | 2.5311           | 0.0000   | 0.1000           | 0.0000  | 1.0000 |
| 2      | Ţ      | 4                   | 73.8008            | 28.9565            | 1.9450           | 0.0000   | 0.2000           | 0.0000  | 2.9066 |
| 1      | 2      | 4                   | 0.0000             | 0.0019             | 6.3000           | 0.0000   | 0.0000           | 0.0000  | 1.0400 |
| 1      | 2<br>2 | ⊥<br>2              | 71.0401            | 45.0000            | 1.2007           | 0.0000   | 2.0294           | 69 1072 | 1 9676 |
| 1      | 2      | 2<br>2              | 70.3000            | 44.0005<br>35 0124 | 2 2286           | 0.0000   | 2 9000           | 0 0000  | 2 4754 |
| ⊥<br>२ | 2      | ד<br>ג              | 89 9293            | 15 8855            | 2.2200           | 0.0000   | 2.9000           | 0.0000  | 1 0237 |
| 3      | 3      | 4                   | 84.0202            | 31.3592            | 1.0534           | 0.0000   | 2.9000           | 0.0000  | 1.4406 |
| 4      | 3      | 4                   | 72.3904            | 15.0722            | 5.0227           | 0.0000   | 3.0072           | 0.0000  | 1.0000 |
| 1      | 3      | 2                   | 90.0000            | 6.6459             | 5.2255           | 0.0000   | 1.3111           | 0.0000  | 3.0000 |
| 2      | 3      | 3                   | 75.6935            | 50.0000            | 2.0000           | 0.0000   | 1.0000           | 0.0000  | 1.1680 |
| 2      | 3      | 4                   | 68.4187            | 33.4407            | 7.5000           | 0.0000   | 0.1000           | 0.0000  | 1.0000 |
| 2      | 3      | 2                   | 85.8000            | 9.8453             | 2.2720           | 0.0000   | 2.8635           | 0.0000  | 1.5800 |
| 1      | 4      | 1                   | 81.2266            | 17.5379            | 1.2324           | 0.0000   | 2.8702           | 0.0000  | 1.0000 |
| 1      | 4      | 3                   | 73.8735            | 39.1639            | 1.0445           | 0.0000   | 2.8701           | 0.0000  | 1.7008 |
| 1      | 4      | 4                   | 71.3629            | 18.4874            | 2.3468           | 0.0000   | 2.8701           | 0.0000  | 1.8255 |
| 3      | 4      | _3<br>⊿             | 74.9080            | 21.9109            | 2.5904           | -18.0069 | 3.0701<br>2.0117 | 0.0000  | 1 0000 |
| 2<br>2 | 4      | 4<br>4              | 76 1795            | 20.9944            | 1 6529           | -0.9193  | 2 9983           | 0.0000  | 2 4525 |
| 1      | 4      | 2                   | 69 0828            | 11 0941            | 2 4635           | 0.0000   | 0 2025           | 0.0000  | 2 3768 |
| 2      | 4      | 3                   | 77.7697            | 23.7768            | 2.7987           | 0.0000   | 0.3956           | 0.0000  | 3.0000 |
| 2      | 4      | 4                   | 74.3012            | 42.0419            | 1.2591           | 0.0000   | 0.5437           | 0.0000  | 1.1369 |
| 2      | 4      | 2                   | 84.3282            | 13.8208            | 4.6573           | 0.0000   | 0.1000           | 0.0000  | 1.0000 |
| 1      | 2      | 3                   | 0.0000             | 16.7302            | 1.1143           | 0.0000   | 0.0000           | 0.0000  | 1.0000 |
| 1      | 2      | 4                   | 0.0000             | 14.7285            | 3.8173           | 0.0000   | 0.0000           | 0.0000  | 2.1043 |
| 1      | 2      | 5                   | 0.0000             | 15.0000            | 3.0000           | 0.0000   | 0.0000           | 0.0000  | 1.0400 |
| 3      | 2      | 3                   | 0.0000             | 15.0000            | 2.8900           | 0.0000   | 0.0000           | 0.0000  | 2.8774 |
| 3      | 2      | 4                   | 0.0000             | 1.4986             | 0.1000           | 0.0000   | 0.0000           | 0.0000  | 3.0000 |
| 4      | 2      | 4                   | 0.0000             | 2.4033             | 0.1000           | 0.0000   | 0.0000           | 0.0000  | 1.8653 |
| 2      | 2      | 3                   | 0.0000             | 8.5/44             | 3.0000           | 0.0000   | 0.0000           | 0.0000  | 1.0421 |
| 1      | 1      | - <del>1</del><br>5 | 74 4180            | 33 4273            | 1 7018           | 0.0000   | 0.0000           | 0.0000  | 1 6178 |
| 1      | 5      | 1                   | 79,7037            | 28,2036            | 1.7073           | 0.1463   | 0.5000           | 0.0000  | 1.6453 |
| 2      | 1      | 5                   | 63.3289            | 29.4225            | 2.1326           | 0.0000   | 0.5000           | 0.0000  | 3.0000 |
| 1      | 5      | 2                   | 85.9449            | 38.3109            | 1.2492           | 0.0000   | 0.5000           | 0.0000  | 1.1000 |
| 1      | 5      | 5                   | 80.0000            | 25.0000            | 2.0000           | 0.0000   | 0.5000           | 0.0000  | 1.3830 |
| 2      | 5      | 2                   | 85.0000            | 15.1317            | 2.0000           | 0.0000   | 0.5000           | 0.0000  | 2.0000 |
| 2      | 5      | 5                   | 97.0064            | 32.1121            | 2.0242           | 0.0000   | 0.5000           | 0.0000  | 2.8568 |
| 2      | 2      | 5                   | 0.0000             | 0.0019             | 6.0000           | 0.0000   | 0.0000           | 0.0000  | 1.0400 |
| 5      | 4      | 5                   | 62.0000            | 33.4273            | 1.7018           | 0.1463   | 0.5000           | 0.0000  | 1.0500 |
| 3      | 5      | 3                   | 77.0699            | 39.4349            | 2.1313           | -30.0000 | 0.9567           | 0.0000  | 1.1483 |
| 1      | 5      | 2<br>2              | 70.0000            | 35.0000            | 3.4223           | 0.0000   | 1 3550           | 0.0000  | 1 2002 |
| 3      | 5      | 4                   | 70.0000            | 35,0000            | 3,4223           | 0.0000   | 1.3550           | 0.0000  | 1,2002 |
| 5      | 1      | 7                   | 70.0000            | 35.0000            | 3.4223           | 0.0000   | 1.3550           | 0.0000  | 1.2002 |
| 1      | 3      | 5                   | 73.0990            | 33.8942            | 1.2098           | 0.0000   | 0.8161           | 0.0000  | 1.1776 |
| 3      | 3      | 5                   | 83.9753            | 31.0715            | 3.5590           | 0.0000   | 0.8161           | 0.0000  | 1.1776 |
| 2      | 3      | 5                   | 76.9521            | 20.0000            | 2.0903           | 0.0000   | 1.0000           | 0.0000  | 1.0400 |
| 2      | 6      | 2                   | 0.0000             | 49.8261            | 0.2093           | 0.0000   | 2.0870           | 0.0000  | 2.2895 |
| 2      | 2      | 6                   | 0.0000             | 39.7818            | 3.1505           | 0.0000   | 1.1296           | 0.0000  | 1.1110 |
| 6      | 2      | 6                   | 0.0000             | 0.5047             | 0.8000           | 0.0000   | 0.8933           | 0.0000  | 4.6650 |
| 2      | 6      | 6<br>2              | 0.0000             | 8./03/             | 0.0827           | 0.0000   | 3.559/           | 0.0000  | 1.1198 |
| 5      | 2      | 5                   | 0.0000             | 25 0000            | 8 0000           | 0.0000   | 1 0000           | 0.0000  | 3 0000 |
| 2      | 2      | 6                   | 66.0423            | 5.0000             | 1.0000           | 0.0000   | 1.0000           | 0.0000  | 1.2500 |
| 2      | 6      | 3                   | 0.0000             | 0.5000             | 0.1000           | 0.0000   | 1.0000           | 0.0000  | 3.0000 |
| 3      | 3      | 6                   | 70.0000            | 20.0000            | 1.0000           | 0.0000   | 1.0000           | 0.0000  | 1.2500 |
| 3      | 7      | 3                   | 88.6293            | 18.2614            | 0.8145           | 0.0000   | -0.1780          | 0.0000  | 2.3661 |
| 2      | 3      | 7                   | 75.0000            | 7.8005             | 0.9394           | 0.0000   | 1.3523           | 0.0000  | 1.0400 |
| 3      | 3      | 7                   | 60.0000            | 40.0000            | 4.0000           | 0.0000   | 1.0000           | 0.0000  | 1.0400 |
| 3      | 2      | 7                   | 0.0000             | 10.0000            | 1.0000           | 0.0000   | 1.0000           | 0.0000  | 1.0400 |
| 6      | 3      | 7                   | 41.7798            | 3.5596             | 7.5000           | 0.0000   | -0.2621          | 0.0000  | 1.0400 |
| 1      | 3<br>n | '/<br>''            | 50.6740<br>76 0677 | L3.3258            | 0.1000<br>2 1105 | 0.0000   | _0_0007          | 0.0000  | 1.1254 |
| 1      | 2      | 1                   | /0.00//            | 5.4450             | 2.1103           | 0.0000   | -0.004/          | 0.0000  | ∠.⊥>>0 |

| 2       | 7      | 3        | 75       | .0000       | 25       | .000      | 0    | 2.0      | 000          |          | 0.00           | 00              | 1.0        | 00      | 0            | 0.     | 000         | 00  | 1.      | . 250   | 0        |
|---------|--------|----------|----------|-------------|----------|-----------|------|----------|--------------|----------|----------------|-----------------|------------|---------|--------------|--------|-------------|-----|---------|---------|----------|
| 3       | 7      | 7        | 70       | .0000       | 25       | .000      | 0    | 2.0      | 000          |          | 0.000          | 00              | 1.0        | 00      | 0            | 0.     | 000         | 00  | 1.      | .250    | 0        |
| 3       | 9      | 3        | 96       | .2265       | 4        | .561      | .0 1 | 2.0      | 000          |          | 0.000          | 00              | 0.3        | 21      | 1            | 0.     | 000         | 00  | 1.      | .520    | )4       |
| 3       | 9      | 3        | 0        | .0000       | 9        | .155      | 2    | 7.9      | 919          |          | 0.000          | 00              | 0.1        | 66      | 0            | 0.     | 000         | 00  | 1.      | . 538   | 36       |
| 9       | 3      | 9        | T00      | .0000       | 10       | .106      | 5    | 6.0      | 000          |          |                | 10              | 1.0        | 17      | 1            | 0.     |             | 0   | 3.      | .660    | ) T      |
| 2       | 3      | 9        | 55<br>70 | .041/       | 30       | 0.503     | 0    | 3.9      | 9/9          |          |                | ) ()<br>) ()    | 1.5        | 1 /     | 1<br>0       | 0.     |             | 0   | 1       | 250     | 0        |
| 3       | 9      | 9        | 66       | 7783        | 14       | 314       | 6    | 2.0      | 911          |          |                | ) ()<br>) ()    | 1 0        | 00      | 0            | 0.     | 000         | 0   | 1       | 230     | 10       |
| 3       | 9      | 10       | 96       | .6924       | 9        | .482      | 3    | 5.7      | 883          |          | 0.000          | 00              | 0.2        | 24      | 8            | 0.     | 000         | 0   | 2       | . 264   | 40       |
| 3       | 9      | 10       | 0        | .0000       | 3        | .854      | 9    | 3.7      | 230          |          | 0.000          | 00              | 0.1        | 48      | 2            | 0.     | 000         | 00  | 1.      | .040    | 0        |
| 9       | 10     | 9        | 0        | .0000       | 11       | .233      | 6    | 6.8      | 851          |          | 0.000          | 00              | 1.0        | 00      | 0            | Ο.     | 000         | 0   | 1.      | . 089   | 3        |
| 9       | 9      | 10       | 90       | .0000       | 5        | .081      | 1    | 5.2      | 147          |          | 0.000          | 00              | 1.0        | 00      | 0            | 0.     | 000         | 00  | 1.      | . 853   | 88       |
| 10      | 9      | 10       | 0        | .0100       | 21       | .148      | 2    | 0.3      | 506          |          | 0.000          | 00              | 1.0        | 00      | 0            | 0.     | 000         | 00  | 1.      | .436    | 51       |
| 3       | 2      | 10       | 0        | .0000       | 0        | .010      | 0    | 0.5      | 211          |          | 0.000          | 00              | 0.0        | 00      | 0            | 0.     | 000         | 00  | 1.      | . 385   | 59       |
| 3       | 9      | 4        | 100      | .0000       | 28       | .153      | 2 1  | 12.0     | 000          |          | 0.000          | 00              | 0.2        | 93      | 2            | 0.     | 000         | 00  | 1.      | .648    | 39       |
| 3       | 9      | 4        | 0        | .0000       | 22       | .745      | .7   | 2.9      | 039          |          | 0.000          | 00              | 0.5        | 59      | 3            | 0.     | 000         | 00  | 1.      | .976    | 04<br>70 |
| 4       | 9      | 4        | 87       | .0081       | 27       | .043      | 0    | 3.9      | 135          |          |                | ) ()<br>) ()    | 4.0        | 00      | 0            | 0.     |             | 0   | 1       | .45/    | 8        |
| 9       | 4      | 9        | 100      | .0000       | 10       | 106       | 5    | 5.1      | 000          |          |                | ) ()<br>) ()    | 1 0        | 00      | 0            | 0.     | 000         | 0   | ⊥.<br>२ | 660     | 11       |
| 2       | 4      | 9        | 80       | .0000       | - 10     | .560      | 1    | 3.3      | 645          |          | 0.000          | 00              | 1.5        | 17      | 1            | 0.     | 000         | 0   | 1       | .040    | 0        |
| 3       | 4      | 9        | 70       | .0000       | 30       | .000      | 0    | 2.0      | 000          |          | 0.000          | 00              | 1.0        | 00      | 0            | 0.     | 000         | 0   | 1       | . 250   | 0        |
| 4       | 3      | 9        | 70       | .0000       | 30       | .000      | 0    | 2.0      | 000          |          | 0.000          | 00              | 1.0        | 00      | 0            | Ο.     | 000         | 00  | 1.      | . 250   | 0        |
| 4       | 4      | 9        | 70       | .0000       | 30       | .000      | 0    | 2.0      | 000          |          | 0.000          | 00              | 1.0        | 00      | 0            | 0.     | 000         | 00  | 1.      | . 250   | 0        |
| 4       | 9      | 9        | 66       | .7783       | 14       | .314      | 6    | 0.7      | 911          |          | 0.000          | 00              | 1.0        | 00      | 0            | 0.     | 000         | 00  | 1.      | . 233   | 33       |
| 4       | 9      | 10       | 95       | .2122       | 5        | .709      | 0 1  | 2.0      | 000          |          | 0.000          | 00              | 0.2        | 24      | 8            | 0.     | 000         | 00  | 2       | . 893   | 86       |
| 4       | 9      | 10       | 0        | .0000       | 9        | .005      | 4    | 7.9      | 511          |          | 0.000          | 00              | 0.1        | 48      | 2            | 0.     | 000         | 00  | 1.      | .624    | 5        |
| 4       | 2      | 10       | 0        | .0000       | 15       | .000      | 0    | 2.8      | 900          |          | 0.000          | 00              | 0.0        | 00      | 0            | 0.     | 000         | 00  | 2.      | .877    | 4        |
| 1       | 3      | 9        | 55       | .0000       | 15       | .000      | 0    | 1.0      | 000          |          |                | 10              | 1.0        | 00      | 0            | 0.     |             | 0   | 1       | .500    | 0        |
| ⊥<br>64 | 4      | פ<br>ז ו | Jr o     | 10000       | t D<br>D |           | 1:2+ | 1.U      | +3:2         | + 1      | 0.000<br>:::V1 | JU<br>: 172 : 1 | 1.0        | 21      |              | U.     | 000<br>07 - | i:n | . ⊥<br> | . 500   | 10       |
| 1       | 1      | 1        | 1        | -0.2        | 500      | .34.      | 7453 | 3        | 0.02         | 88       | -6             | .350            | 7 –        | 1.      | 6000         | ) VC   | 0.          | 000 | 0       | 0.      | 0000     |
| 1       | 1      | 1        | 2        | -0.2        | 500      | 29.       | 2131 | Ĺ        | 0.29         | 45       | -4             | .9581           | L –        | 2.      | 1802         | 2      | 0.          | 000 | 0       | 0.      | 0000     |
| 2       | 1      | 1        | 2        | -0.2        | 500      | 31.       | 2081 | L        | 0.45         | 39       | -4             | .8923           | 3 –        | 2.      | 2677         | 7      | 0.          | 000 | 0       | 0.      | 0000     |
| 1       | 1      | 1        | 3        | -2.5        | 000      | 25.       | 4016 | 5        | 1.00         | 00       | -4             | .4850           | ) –        | 1.      | 1000         | )      | 0.          | 000 | 0       | 0.      | 0000     |
| 2       | 1      | 1        | 3        | -0.9        | 763      | 59.       | 4161 | L        | 1.00         | 00       | -7             | .7414           | 4 –        | 1.      | 0978         | 3      | 0.          | 000 | 0       | 0.      | 0000     |
| 3       | 1      | 1        | 3        | -2.5        | 000      | 52.       | 7614 | 1 –      | 1.00         | 00       | -4             | .0134           | 4 –        | Ο.      | 8614         | ł      | 0.          | 000 | 0       | 0.      | 0000     |
| 1       | 1      | 3        | 1        | -1.9        | 125      | 80.       | 0000 | ) –      | 1.00         | 00       | -4             | .5626           | 5 -        | 0.      | 9000         | )      | 0.          | 000 | 0       | 0.      | 0000     |
| 1       | 1      | 3        | 2        | 0.6         | 154      | 8.        | 3019 | ) –      | 0.48         | 70       | -2             | .9336           | - c        | 0.      | 9000         | )      | 0.          | 000 | 0       | 0.      | 0000     |
| 2       | 1      | 3        | ⊥<br>2   | -2.5        | 000      | 80.<br>31 | 8695 | 5        | 1 00         | 58<br>00 | -4             | 6151            | - c<br>1 _ | 1       | 9000<br>1000 | ,<br>) | 0.          | 000 | 0       | 0.      | 0000     |
| 1       | 1      | 2        | 2        | 0 7         | 514      | 34        | 1941 | ,        | 0 56         | 69       | -5             | 5360            | י<br>ר     | 2       | 0544         | ,<br>L | 0.          | 000 | 0       | 0.      | 0000     |
| 2       | 1      | 3        | 3        | 2.5         | 000      | 80.       | 0000 | )        | 1.00         | 00       | -2             | .6841           | ,<br>1 –   | 2.      | 8274         | -      | 0.          | 000 | 0       | 0.      | 0000     |
| 3       | 1      | 3        | 1        | 0.2         | 515      | 79.       | 1495 | 5 –      | 0.62         | 63       | -4             | .3647           | -<br>7 -   | 3.      | 0437         | ,      | 0.          | 000 | 0       | 0.      | 0000     |
| 3       | 1      | 3        | 2        | 1.0         | 000      | 37.       | 1243 | 3        | 1.00         | 00       | -2             | .5000           | ) –        | 3.      | 0476         | 5      | 0.          | 000 | 0       | 0.      | 0000     |
| 3       | 1      | 3        | 3        | -1.0        | 092      | 41.       | 0504 | ł        | 0.39         | 15       | -б             | .0913           | 3 –        | 2.      | 7174         | Ł      | 0.          | 000 | 0       | 0.      | 0000     |
| 1       | 3      | 3        | 1        | -1.6        | 378      | -11.      | 8357 | 7        | 0.38         | 15       | -3             | .2104           | 4 –        | 2.      | 7536         | ,      | 0.          | 000 | 0       | 0.      | 0000     |
| 1       | 3      | 3        | 2        | -2.5        | 000      | -9.       | 2805 | 5        | 0.30         | 63       | -5             | .918            | 7 –        | 2.      | 9498         | 3      | 0.          | 000 | 0       | 0.      | 0000     |
| 2       | 3      | 3        | 2        | 0.2         | 732      | -21.      | 6925 | o –      | 1.00         | 00       | -2             | .5000           | ) –        | 0.      | 9921         | -      | 0.          | 000 | 0       | 0.      | 0000     |
| 1<br>2  | 3      | 3        | 3        | ∠.5<br>_2.5 | 000      | -1/.      | 0041 |          | 1.00         |          | -2             | .5000           | – נ<br>כ   | U.<br>1 | 9972<br>2405 | ,      | 0.          | 000 | 0       | 0.      | 0000     |
| 2       | 2      | 2        | 2        | -2.5        | 000      | -25       | 0000 | , –<br>, | 1 00         | 00       | -2             | 5000            | 2 –<br>) _ | 1.<br>0 | 2407<br>9000 | )      | 0.          | 000 | 0       | 0.      | 0000     |
| 1       | 1      | 4        | 2        | 1.4         | 427      | 31        | 7903 | 3        | 0.20         | 54       | -8             | . 0000          | ) _        | 1.      | 9825         | 5      | 0.          | 000 | 0       | 0.      | 0000     |
| 2       | 1      | 4        | 2        | -1.0        | 000      | 64.       | 2008 | 3        | 0.30         | 37       | -7             | .5233           | 3 –        | 2.      | 1051         |        | 0.          | 000 | 0       | 0.      | 0000     |
| 3       | 1      | 4        | 2        | 1.0         | 000      | 29.       | 1410 | )        | 1.00         | 00       | -3             | .2244           | 4 –        | 2.      | 5261         |        | 0.          | 000 | 0       | 0.      | 0000     |
| 3       | 1      | 1        | 4        | -1.0        | 000      | 65.       | 1457 | 7        | 0.24         | 33       | -4             | .9542           | 2 –        | Ο.      | 9511         | -      | 0.          | 000 | 0       | 0.      | 0000     |
| 4       | 1      | 1        | 4        | 1.0         | 000      | 87.       | 8413 | 3        | 0.38         | 17       | -3             | .7479           | 9 -        | 1.      | 7241         | -      | 0.          | 000 | 0       | 0.      | 0000     |
| 1       | 1      | 4        | 1        | 1.0         | 000      | 12.       | 2873 | 3        | 0.74         | 38       | -3             | .5510           | ) –        | 1.      | 6589         | )      | 0.          | 000 | 0       | 0.      | 0000     |
| 3       | 1      | 4        | 1        | -1.0        | 000      | -0.       | 2183 | 3        | 1.00         | 00       | -3             | .5014           | 4 –        | 1.      | 8038         | 3      | 0.          | 000 | 0       | 0.      | 0000     |
| 2       | 1      | 1        | 4        | 1.0         | 000      | 23.       | 7736 | 5        | 0.42         | 35       | -2             | .7665           | 5 -        | 1.      | 9000         | )      | 0.          | 000 | 0       | 0.      | 0000     |
| 4<br>2  | 1      | 4        | 2        | 1.0<br>_1 0 | 000      | 96.       | 1436 | 7        | 1.00<br>1.00 | 00<br>20 | -6             | .9528           | 5 –<br>5   | ∠.<br>1 | U202         | 1      | υ.          | 000 | 0       | 0.      | 0000     |
| ⊿<br>∩  | ⊥<br>1 | 4<br>2   | U<br>T   | 0.1-        | 000      | 00.<br>N  | 0000 | , –<br>) | 0.34         | 33<br>00 | - / .          | , 2006<br>1000  | י –<br>ר   | 1.<br>0 | 0000         | ,<br>) | 0.          | 000 | 0       | 0.<br>N | 0000     |
| 0       | ⊥<br>2 | ∠<br>2   | n        | 0.0         | 000      | 0.        | 0000 | ,<br>)   | 0.00         | 00       | 0              |                 | 5          | 0.      | 0000         | ,<br>) | 0.          | 000 | 0       | 0.      | 0000     |
| 0       | 2      | 3        | 0        | 0.0         | 000      | 0         | 1000 | )        | 0.02         | 00       | -2             | .541            | -          | 0.      | 0000         | )      | 0           | 000 | õ       | 0       | 0000     |
| 0       | 1      | 1        | Õ        | 0.0         | 000      | 50.       | 0000 | )        | 0.30         | 00       | -4             | .0000           | -<br>D —   | 2.      | 0000         | )      | 0.          | 000 | 0       | 0.      | 0000     |
| 0       | 3      | 3        | 0        | 0.5         | 511      | 25.       | 4150 | )        | 1.13         | 30       | -5             | .1903           | 3 –        | 1.      | 0000         | )      | 0.          | 000 | 0       | 0.      | 0000     |
| 0       | 1      | 4        | 0        | 0.2         | 176      | 40.       | 4126 | 5        | 0.35         | 35       | -3             | .9875           | 5 -        | 2.      | 0051         | -      | 0.          | 000 | 0       | 0.      | 0000     |
| 0       | 2      | 4        | 0        | 0.0         | 000      | 0.        | 1032 | 2        | 0.30         | 00       | -5             | .0965           | 5          | 0.      | 0000         | )      | 0.          | 000 | 0       | 0.      | 0000     |
| 0       | 3      | 4        | 0        | 1.1         | 397      | 61.       | 3225 | 5        | 0.51         | 39       | -3             | .850            | 7 –        | 2.      | 7831         | -      | 0.          | 000 | 0       | 0.      | 0000     |

| 0 | 4 | 4   | 0   | 0.726   | 55 44.315  | 5 1.000   | 0 -4.4046  | 5 -2.0000 | 0.0000 | 0.0000 |
|---|---|-----|-----|---------|------------|-----------|------------|-----------|--------|--------|
| 4 | 1 | 4   | 4   | -0.094  | 19 8.758   | 0.331     | .0 -7.9430 | -2.0000   | 0.0000 | 0.0000 |
| 0 | 1 | 5   | 0   | 0.825   | 51 92.146  | 58 0.717  | /6 -4.2341 | L 0.0000  | 0.0000 | 0.0000 |
| 0 | 5 | 5   | 0   | 0.129   | 91 -5.000  | 0.964     | 49 -5.0903 | 3 0.0000  | 0.0000 | 0.0000 |
| 0 | 2 | 5   | 0   | 0.000   | 0.000      | 0.000     | 0.0000     | 0.0000    | 0.0000 | 0.0000 |
| 0 | б | б   | 0   | 0.000   | 0.000      | 0.120     | 0 -2.4426  | 5 0.0000  | 0.0000 | 0.0000 |
| 0 | 2 | б   | 0   | 0.000   | 0.000      | 0.120     | 0 -2.4847  | 7 0.0000  | 0.0000 | 0.0000 |
| 0 | 3 | б   | 0   | 0.000   | 0.000      | 0.120     | 0 -2.4703  | 3 0.0000  | 0.0000 | 0.0000 |
| 1 | 1 | 3   | 3   | -0.000  | 20.185     | 51 0.160  | )1 -9.0000 | -2.0000   | 0.0000 | 0.0000 |
| 1 | 3 | 3   | 1   | 0.000   | 2 80.000   | 0 -1.500  | 0 -4.4848  | 3 -2.0000 | 0.0000 | 0.0000 |
| 3 | 1 | 3   | 3   | -0.158  | 33 20.000  | 0 1.500   | 00 -9.0000 | -2.0000   | 0.0000 | 0.0000 |
| 1 | 1 | 1   | 7   | 0.000   | 0 19.387   | 1 0.010   | 3 -25.5765 | 5 -1.7255 | 0.0000 | 0.0000 |
| 7 | 1 | 1   | 7   | 0.000   | 0 80.558   | 0.110     | 4 -8.0928  | 3 -1.7255 | 0.0000 | 0.0000 |
| 0 | 1 | 7   | 0   | 4.000   | 0 45.826   | 54 0.900  | 00 -4.0000 | 0.0000    | 0.0000 | 0.0000 |
| 0 | 7 | 7   | 0   | 4.000   | 0 45.826   | 54 0.900  | 00 -4.0000 | 0.0000    | 0.0000 | 0.0000 |
| 2 | 1 | 3   | 7   | -1.500  | 00 13.748  | .171      | .0 -3.7686 | 5 0.0000  | 0.0000 | 0.0000 |
| 2 | 3 | 7   | 3   | -0.312  | 20 -1.799  | 0.237     | /1 -3.2710 | 0.0000    | 0.0000 | 0.0000 |
| 1 | 3 | 7   | 3   | -1.500  | 0 -2.500   | 0.679     | 94 -2.5000 | 0.0000    | 0.0000 | 0.0000 |
| 7 | 3 | 7   | 3   | -1.500  | 0 7.460    | 0 -0.907  | /5 -9.0000 | 0.0000    | 0.0000 | 0.0000 |
| 2 | 3 | 9   | 3   | -1.500  | 6.833      | 3 -0.197  | /8 -1.4683 | 3 0.0000  | 0.0000 | 0.0000 |
| 2 | 3 | 9   | 4   | -0.618  | 31 7.154   | 2 -0.004  | 47 -1.6577 | 7 0.0000  | 0.0000 | 0.0000 |
| 2 | 4 | 9   | 3   | -1.500  | 0 1.782    | 20 -1.000 | 0 -5.4916  | 5 0.0000  | 0.0000 | 0.0000 |
| 2 | 4 | 9   | 4   | -0.195  | 59 2.362   | 26 -1.000 | 0 -3.0702  | 2 0.0000  | 0.0000 | 0.0000 |
| 2 | 1 | 4   | 9   | 0.000   | 00 10.000  | 0.300     | 00 -6.0000 | 0 -1.0000 | 0.0000 | 0.0000 |
| 2 | 3 | 9   | 10  | 0.158   | 39 12.500  | 0.438     | 88 -1.5000 | 0.0000    | 0.0000 | 0.0000 |
| 9 |   | ! N | r o | f hydro | ogen bonds | ;at1;at2; | at3;Rhb;De | hb;vhb1   |        |        |
| 3 | 2 | 3   | 2   | .1200   | -3.5800    | 1.4500    | 19.5000    |           |        |        |
| 3 | 2 | 4   | 2   | .0985   | -4.5000    | 1.4500    | 19.5000    |           |        |        |
| 4 | 2 | 3   | 1   | .7500   | -1.5000    | 1.4500    | 19.5000    |           |        |        |
| 4 | 2 | 4   | 1   | .9893   | -3.2987    | 1.4500    | 19.5000    |           |        |        |
| 3 | 2 | 5   | 1   | .5000   | -2.0000    | 1.4500    | 19.5000    |           |        |        |
| 4 | 2 | 5   | 1   | .5000   | -2.0000    | 1.4500    | 19.5000    |           |        |        |
| 5 | 2 | 3   | 1   | .5000   | -2.0000    | 1.4500    | 19.5000    |           |        |        |
| - | 0 | 4   | 1   | F000    | 0 0000     | 1 4500    | 10 5000    |           |        |        |

5241.5000-2.00001.450019.50005251.5000-2.00001.450019.5000

| Atom | r <sub>o</sub> | χ <sub>EEM</sub> (eV)    | η <sub>εεм</sub> (eV)         | γεεμ              | r <sub>vdW</sub> | EvdW                     | $\alpha_{vdW}$ | γvdW    |
|------|----------------|--------------------------|-------------------------------|-------------------|------------------|--------------------------|----------------|---------|
|      | $r_{\pi}$      | $r_{\pi\pi}$             |                               |                   |                  |                          |                |         |
| С    | 1.3817         | 6.0000                   | 4.9218                        | 0.6387            | 1.8903           | 0.1838                   | 9.7559         | 2.1346  |
|      | 1.1341         | 1.2114                   |                               |                   |                  |                          |                |         |
| Н    | 0.8930         | 9.6093                   | 3.7248                        | 0.8203            | 1.3550           | 0.0930                   | 8.2230         | 33.2894 |
|      | _              | _                        |                               |                   |                  |                          |                |         |
| 0    | 1.2450         | 8.3122                   | 8.5000                        | 1.0898            | 2.3890           | 0.1000                   | 9.7300         | 13.8449 |
|      | 1.0548         | 0.9049                   |                               |                   |                  |                          |                |         |
| Ν    | 1.2333         | 7.0317                   | 6.4603                        | 1.0000            | 2.1294           | 0.1322                   | 10.0056        | 10.8657 |
|      | 1.1748         | 1.0433                   |                               |                   |                  |                          |                |         |
| S    | 1.9673         | 8.2545                   | 6.5000                        | 1.0336            | 2.1729           | 0.3000                   | 10.3008        | 4.9055  |
|      | 1.5359         | 1.4601                   |                               |                   |                  |                          |                |         |
| Bond |                | $p_{\it be,1}$           | p <sub>ovun,1</sub>           | p <sub>be,2</sub> | $p_{bo,1}$       | <b>р</b> <sub>bo,2</sub> |                |         |
|      |                | <b>р</b> <sub>bo,3</sub> | $p_{\scriptscriptstyle bo,4}$ |                   | $p_{bo,5}$       | $p_{bo,6}$               |                |         |
| C-C  | 158.2004       | -0.7738                  | 0.4147                        | 0.4590            | -0.0777          | 6.7268                   |                |         |
|      | 99.1897        | -0.1000                  | 9.1628                        | 78.0000           | -0.4550          | 37.6117                  |                |         |
| C-H  | 169.4760       | -0.6083                  | 0.7652                        | 5.2290            | -0.0553          | 6.9316                   |                |         |
|      | 0.0000         | _                        | _                             | 0.0000            | _                | _                        |                |         |
| H-H  | 153.3934       | -0.4600                  | 0.7300                        | 6.2500            | -0.0790          | 6.0552                   |                |         |
|      | 0.0000         | _                        | _                             | 0.0000            | _                | _                        |                |         |
| C-0  | 115.3161       | 0.5141                   | 0.9954                        | 1.5618            | -0.1628          | 5.6821                   |                |         |
|      | 127.1562       | -0.3414                  | 8.9489                        | 61.7072           | -0.3474          | 18.9948                  |                |         |
| 0-0  | 142.2858       | 0.2506                   | 0.6051                        | 0.3451            | -0.1225          | 5.5000                   |                |         |
|      | 145.0000       | -0.1055                  | 9.0000                        | 50.8293           | -0.1000          | 29.7503                  |                |         |
| C-N  | 164.1304       | -1.8021                  | 0.2487                        | 0.3953            | -0.2557          | 4.6940                   |                |         |
|      | 141.3380       | -0.3663                  | 7.1330                        | 102.0464          | -0.5696          | 27.6095                  |                |         |
| O-N  | 128.8596       | 0.3819                   | 0.1900                        | 1.0110            | -0.1265          | 6.8843                   |                |         |
|      | 167.8643       | -0.3716                  | 7.0805                        | 40.0000           | -0.1539          | 34.9972                  |                |         |
| N-N  | 160.1592       | 0.4110                   | 0.5899                        | 0.1538            | -0.0753          | 5.4371                   |                |         |
|      | 82.5526        | -0.1473                  | 11.9187                       | 153.9884          | -0.0934          | 12.4304                  |                |         |
| H-O  | 160.0000       | -0.5725                  | 0.5626                        | 1.1150            | -0.0920          | 4.2790                   |                |         |
|      | 0.0000         | _                        | _                             | 0.0000            | _                | _                        |                |         |
| H-N  | 211.6032       | -0.3415                  | 0.4726                        | 2.7198            | -0.1744          | 5.6399                   |                |         |
|      | 0.0000         | _                        | _                             | 0.0000            | _                | _                        |                |         |
| C-S  | 150.8132       | -0.0628                  | 0.3219                        | 0.3317            | -0.1946          | 5.9455                   |                |         |
|      | 59.3363        | -0.2289                  | 7.5946                        | 55.2528           | -0.5211          | 18.9617                  |                |         |
| H-S  | 143.4377       | -0.2944                  | 0.6034                        | 9.5627            | -0.0516          | 7.0960                   |                |         |
|      | 0.0000         | _                        | _                             | 0.0000            | _                | _                        |                |         |

Table 1: ReaxFF parameters for the protein force field – units are in Ångstrom, degrees and kcal/mol, unless mentioned otherwise.

| O-S           | 0.0000        | 0.5563    | 0.6000         | 0.4259                 | -0.1100            | 7.1145           |
|---------------|---------------|-----------|----------------|------------------------|--------------------|------------------|
|               | 0.0000        | -0.4577   | 12.7569        | 0.0000                 | _                  | _                |
| N-S           | 0.0000        | 0.4438    | 0.6000         | 0.3296                 | -0.1805            | 5.6864           |
|               | 0.0000        | -0.3153   | 9.1227         | 0.0000                 | _                  | _                |
| S-S           | 140.8887      | -0.4111   | -0.1336        | 0.2881                 | -0.1806            | 7.4732           |
|               | 84.9350       | -0.2494   | 9.8436         | 68.6860                | -0.4781            | 17.8574          |
| Off-Diagonal  | $r^{\square}$ | $r^{\pi}$ | $r^{\pi\pi}$   | <i>r<sub>vdW</sub></i> | $\alpha_{vdW}$     | ε <sub>vdW</sub> |
| C-H           | 1.1210        | _         | _              | 1.4004                 | 9.8467             | 0.1239           |
| H-O           | 0.9215        | _         | _              | 1.2885                 | 10.9190            | 0.0283           |
| H-N           | 1.0569        | _         | _              | 1.3100                 | 9.6406             | 0.1664           |
| C-0           | 1.3492        | 1.1992    | 1.0506         | 1.8006                 | 10.2114            | 0.0503           |
| C-N           | 1.3428        | 1.2492    | 1.1154         | 1.8995                 | 9.6891             | 0.1771           |
| O-N           | 1.4587        | 1.0933    | 1.1826         | 1.8388                 | 9.5137             | 0.2000           |
| C-S           | 1.7489        | 1.3150    | 1.4031         | 1.7943                 | 10.1042            | 0.1618           |
| H-S           | 1.4206        | _         | _              | 1.5838                 | 10.1462            | 0.0764           |
| O-S           | 1.5799        | 1.4000    | _              | 1.9887                 | 10.0605            | 0.1022           |
| N-S           | 1.8000        | 1.4000    | _              | 1.9000                 | 10.5104            | 0.1505           |
| Valence Angle | θο            | ka        | k <sub>b</sub> | $p_{val,1}$            | p <sub>val,2</sub> |                  |
| C-C-C         | 59.0573       | 30.7029   | 0.7606         | 0.7180                 | 1.1244             |                  |
| C-C-H         | 65.7758       | 14.5234   | 6.2481         | 0.5665                 | 1.6255             |                  |
| H-C-H         | 70.2607       | 25.2202   | 3.7312         | 0.0050                 | 2.7500             |                  |
| C-H-H         | 0.0000        | 0.0000    | 6.0000         | 0.0000                 | 1.0400             |                  |
| C-H-C         | 0.0000        | 3.4110    | 7.7350         | 0.0000                 | 1.0400             |                  |
| H-H-H         | 0.0000        | 27.9213   | 5.8635         | 0.0000                 | 1.0400             |                  |
| C-C-O         | 54.7427       | 21.1992   | 1.0613         | 2.9950                 | 1.1232             |                  |
| 0-C-0         | 78.6632       | 16.3065   | 6.3613         | 1.5183                 | 2.2234             |                  |
| C-C-N         | 78.9895       | 29.7448   | 1.4146         | 1.1834                 | 2.4298             |                  |
| O-C-N         | 74.5431       | 30.9283   | 1.2618         | 1.1019                 | 1.0888             |                  |
| N-C-N         | 90.0000       | 15.9388   | 0.5081         | 1.1155                 | 2.5891             |                  |
| H-C-O         | 50.0000       | 12.9103   | 2.5311         | 0.1000                 | 1.0000             |                  |
| H-C-N         | 73.8008       | 28.9565   | 1.9450         | 0.2000                 | 2.9066             |                  |
| C-H-N         | 0.0000        | 0.0019    | 6.3000         | 0.0000                 | 1.0400             |                  |
| C-O-C         | 71.6401       | 45.0000   | 1.2667         | 2.8294                 | 1.0000             |                  |
| C-O-O         | 76.3686       | 44.8665   | 1.9461         | 1.0572                 | 1.8676             |                  |
| C-O-N         | 70.4701       | 35.0124   | 2.2286         | 2.9000                 | 2.4754             |                  |
| 0-0-0         | 89.9293       | 15.8855   | 2.0229         | 2.9881                 | 1.0237             |                  |
| 0-0-N         | 84.0202       | 31.3592   | 1.0534         | 2.9000                 | 1.4406             |                  |
| N-O-N         | 72.3904       | 15.0722   | 5.0227         | 3.0072                 | 1.0000             |                  |
| С-О-Н         | 90.0000       | 6.6459    | 5.2255         | 1.3111                 | 3.0000             |                  |
| H-O-O         | 75.6935       | 50.0000   | 2.0000         | 1.0000                 | 1.1680             |                  |

| H-O-N         | 68.4187        | 33.4407        | 7.5000         | 0.1000             | 1.0000             |
|---------------|----------------|----------------|----------------|--------------------|--------------------|
| H-O-H         | 85.8000        | 9.8453         | 2.2720         | 2.8635             | 1.5800             |
| C-N-C         | 81.2266        | 17.5379        | 1.2324         | 2.8702             | 1.0000             |
| C-N-O         | 73.8735        | 39.1639        | 1.0445         | 2.8701             | 1.7008             |
| C-N-N         | 71.3629        | 18.4874        | 2.3468         | 2.8701             | 1.8255             |
| 0-N-0         | 74.9086        | 21.9109        | 2.5904         | 3.0701             | 1.0000             |
| O-N-N         | 77.8757        | 28.9944        | 1.2740         | 3.0117             | 1.0000             |
| N-N-N         | 76.1795        | 29.2290        | 1.6529         | 2.9983             | 2.4525             |
| C-N-H         | 69.0828        | 11.0941        | 2.4635         | 0.2025             | 2.3768             |
| H-N-O         | 77.7697        | 23.7768        | 2.7987         | 0.3956             | 3.0000             |
| H-N-N         | 74.3012        | 42.0419        | 1.2591         | 0.5437             | 1.1369             |
| H-N-H         | 84.3282        | 13.8208        | 4.6573         | 0.1000             | 1.0000             |
| C-H-O         | 0.0000         | 16.7302        | 1.1143         | 0.0000             | 1.0000             |
| C-H-N         | 0.0000         | 14.7285        | 3.8173         | 0.0000             | 2.1043             |
| C-H-S         | 0.0000         | 15.0000        | 3.0000         | 0.0000             | 1.0400             |
| O-H-O         | 0.0000         | 15.0000        | 2.8900         | 0.0000             | 2.8774             |
| O-H-N         | 0.0000         | 1.4986         | 0.1000         | 0.0000             | 3.0000             |
| N-H-N         | 0.0000         | 2.4033         | 0.1000         | 0.0000             | 1.8653             |
| H-H-O         | 0.0000         | 8.5744         | 3.0000         | 0.0000             | 1.0421             |
| H-H-N         | 0.0000         | 0.0019         | 6.0000         | 0.0000             | 1.0400             |
| C-C-S         | 74.4180        | 33.4273        | 1.7018         | 0.5000             | 1.6178             |
| C-S-C         | 79.7037        | 28.2036        | 1.7073         | 0.5000             | 1.6453             |
| H-C-S         | 63.3289        | 29.4225        | 2.1326         | 0.5000             | 3.0000             |
| C-S-H         | 85.9449        | 38.3109        | 1.2492         | 0.5000             | 1.1000             |
| C-S-S         | 80.0000        | 25.0000        | 2.0000         | 0.5000             | 1.3830             |
| H-S-H         | 85.0000        | 15.1317        | 2.0000         | 0.5000             | 2.0000             |
| H-S-S         | 97.0064        | 32.1121        | 2.0242         | 0.5000             | 2.8568             |
| H-H-S         | 0.0000         | 0.0019         | 6.0000         | 0.0000             | 1.0400             |
| S-N-S         | 62.0000        | 33.4273        | 1.7018         | 0.5000             | 1.0500             |
| 0-S-0         | 77.0699        | 39.4349        | 2.1313         | 0.9567             | 1.1483             |
| C-S-O         | 70.0000        | 35.0000        | 3.4223         | 1.3550             | 1.2002             |
| C-S-N         | 70.0000        | 35.0000        | 3.4223         | 1.3550             | 1.2002             |
| N-C-S         | 60.0000        | 35.0000        | 3.0223         | 2.3550             | 1.2002             |
| O-S-N         | 70.0000        | 35.0000        | 3.4223         | 1.3550             | 1.2002             |
| C-O-S         | 73.0990        | 33.8942        | 1.2098         | 0.8161             | 1.1776             |
| 0-0-S         | 83.9753        | 31.0715        | 3.5590         | 0.8161             | 1.1776             |
| H-O-S         | 76.9521        | 20.0000        | 2.0903         | 1.0000             | 1.0400             |
| Torsion Angle | V <sub>1</sub> | V <sub>2</sub> | V <sub>3</sub> | p <sub>tor,1</sub> | p <sub>tor,2</sub> |
| C-C-C-C       | -0.2500        | 34.7453        | 0.0288         | -6.3507            | -1.6000            |
| C-C-C-H       | -0.2500        | 29.2131        | 0.2945         | -4.9581            | -2.1802            |

| H-C-C-H | -0.2500 | 31.2081  | 0.4539  | -4.8923 | -2.2677 |
|---------|---------|----------|---------|---------|---------|
| C-C-C-O | -2.5000 | 25.4016  | 1.0000  | -4.4850 | -1.1000 |
| H-C-C-O | -0.9763 | 59.4161  | 1.0000  | -7.7414 | -1.0978 |
| 0-C-C-0 | -2.5000 | 52.7614  | -1.0000 | -4.0134 | -0.8614 |
| C-C-O-C | -1.9125 | 80.0000  | -1.0000 | -4.5626 | -0.9000 |
| С-С-О-Н | 0.6154  | 8.3019   | -0.4870 | -2.9336 | -0.9000 |
| Н-С-О-С | -2.5000 | 80.0000  | 0.9658  | -4.4935 | -0.9000 |
| H-C-O-H | -1.0000 | 31.8695  | 1.0000  | -2.6151 | -1.1000 |
| C-C-O-O | 0.7514  | 34.1941  | 0.5669  | -5.5360 | -2.0544 |
| H-C-O-O | 2.5000  | 80.0000  | 1.0000  | -2.6841 | -2.8274 |
| 0-C-0-C | 0.2515  | 79.1495  | -0.6263 | -4.3647 | -3.0437 |
| О-С-О-Н | 1.0000  | 37.1243  | 1.0000  | -2.5000 | -3.0476 |
| 0-C-0-0 | -1.0092 | 41.0504  | 0.3915  | -6.0913 | -2.7174 |
| C-O-O-C | -1.6378 | -11.8357 | 0.3815  | -3.2104 | -2.7536 |
| С-О-О-Н | -2.5000 | -9.2805  | 0.3063  | -5.9187 | -2.9498 |
| Н-О-О-Н | 0.2732  | -21.6925 | -1.0000 | -2.5000 | -0.9921 |
| C-O-O-O | 2.5000  | -17.6041 | 1.0000  | -2.5000 | -0.9972 |
| H-O-O-O | -2.5000 | 78.0855  | -0.8750 | -7.8902 | -1.2407 |
| 0-0-0-0 | -2.5000 | -25.0000 | 1.0000  | -2.5000 | -0.9000 |
| C-C-N-H | 1.4427  | 31.7903  | 0.2054  | -8.0000 | -1.9825 |
| H-C-N-H | -1.0000 | 64.2008  | 0.3037  | -7.5233 | -2.1051 |
| O-C-N-H | 1.0000  | 29.1410  | 1.0000  | -3.2244 | -2.5261 |
| O-C-C-N | -1.0000 | 65.1457  | 0.2433  | -4.9542 | -0.9511 |
| N-C-C-N | 1.0000  | 87.8413  | 0.3817  | -3.7479 | -1.7241 |
| C-C-N-C | 1.0000  | 12.2873  | 0.7438  | -3.5510 | -1.6589 |
| O-C-N-C | -1.0000 | -0.2183  | 1.0000  | -3.5014 | -1.8038 |
| H-C-C-N | 1.0000  | 23.7736  | 0.4235  | -2.7665 | -1.9000 |
| N-C-N-H | 1.0000  | 96.1436  | 1.0000  | -6.9528 | -2.0202 |
| H-C-N-C | -1.0000 | 88.5527  | -0.3433 | -7.9806 | -1.5996 |
| X-C-H-X | 0.0000  | 0.0000   | 0.0000  | 0.0000  | 0.0000  |
| Х-Н-Н-Х | 0.0000  | 0.0000   | 0.0000  | 0.0000  | 0.0000  |
| X-H-O-X | 0.0000  | 0.1000   | 0.0200  | -2.5415 | 0.0000  |
| X-C-C-X | 0.0000  | 50.0000  | 0.3000  | -4.0000 | -2.0000 |
| X-O-O-X | 0.5511  | 25.4150  | 1.1330  | -5.1903 | -1.0000 |
| X-C-N-X | 0.2176  | 40.4126  | 0.3535  | -3.9875 | -2.0051 |
| X-H-N-X | 0.0000  | 0.1032   | 0.3000  | -5.0965 | 0.0000  |
| X-O-N-X | 1.1397  | 61.3225  | 0.5139  | -3.8507 | -2.7831 |
| X-N-N-X | 0.7265  | 44.3155  | 1.0000  | -4.4046 | -2.0000 |
| N-C-N-N | -0.0949 | 8.7582   | 0.3310  | -7.9430 | -2.0000 |
| X-C-S-X | 0.8251  | 92.1468  | 0.7176  | -4.2341 | 0.0000  |

| VCCV    | 0 1 2 0 1              | F 0000         | 0.0640     | F 0002                   | 0 0000  |
|---------|------------------------|----------------|------------|--------------------------|---------|
| 8-2-2-8 | 0.1291                 | -5.0000        | 0.9649     | -5.0903                  | 0.0000  |
| X-H-S-X | 0.0000                 | 0.0000         | 0.0000     | 0.0000                   | 0.0000  |
| C-C-O-O | -0.0002                | 20.1851        | 0.1601     | -9.0000                  | -2.0000 |
| C-O-O-C | 0.0002                 | 80.0000        | -1.5000    | -4.4848                  | -2.0000 |
| 0-C-0-0 | -0.1583                | 20.0000        | 1.5000     | -9.0000                  | -2.0000 |
| H-Bond  | <b>r</b> <sub>hb</sub> | D <sub>e</sub> | $p_{hb,1}$ | <b>p</b> <sub>hb,2</sub> |         |
| О-Н-О   | 2.1200                 | -3.5800        | 1.4500     | 19.5000                  |         |
| O-H-N   | 2.0985                 | -4.5000        | 1.4500     | 19.5000                  |         |
| N-H-O   | 1.7500                 | -1.5000        | 1.4500     | 19.5000                  |         |
| N-H-N   | 1.9893                 | -3.2987        | 1.4500     | 19.5000                  |         |
| O-H-S   | 1.5000                 | -2.0000        | 1.4500     | 19.5000                  |         |
| N-H-S   | 1.5000                 | -2.0000        | 1.4500     | 19.5000                  |         |
| S-H-O   | 1.5000                 | -2.0000        | 1.4500     | 19.5000                  |         |
| S-H-N   | 1.5000                 | -2.0000        | 1.4500     | 19.5000                  |         |
| S-H-S   | 1.5000                 | -2.0000        | 1.4500     | 19.5000                  |         |