SUPPORTING INFORMATION -A REGRESSION APPROACH TO ACCURATE INTERACTION ENERGIES USING TOPOLOGICAL DESCRIPTORS

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1.1 Cross-validation

k-fold cross-validation was used to ensure the homogeneity of the training set. The value of k was set to 5. Results are presented in the following table.

subset	score
1	0.997
2	0.996
3	0.995
4	0.994
5	0.997

Table 1.1: Scores for the cross-validation of the training set.

The final accuracy is of 0.996 ± 0.001.

1.2 Training and test scores

The training and test scores obtained with the four functionals are reported in the following Table. The consistent and high score in training and test indicates that the algorithm is not overfitting.

functional	score training	score test
PBE	0.986	0.988
PBE-D3	0.995	0.996
B3LYP-D3	0.997	0.997
M06-2X	0.992	0.995

Table 1.2: Training and test score for the kernel Ridge regression with the four functionals

1.3 Comparison of kernel and linear Ridge Regression

The training and test scores obtained for the B3LYP-D3, PBE-D3, M06-2X and PBE functionals in both the kernel and a linear Ridge regression are presented.

functional	score training K	score test K	score training L	score test L
B3LYP-D3	0.997	0.997	0.990	0.993
PBE-D3	0.995	0.996	0.983	0.985
M062X	0.992	0.995	0.982	0.986
PBE	0.986	0.988	0.969	0.972

Table 1.3: Training and test scores obtained with the kernel Ridge regression compared with those of a linear regression.

The coefficients of the linear regression are shown in Table 1.4.

functional	int -0.1 to -0.02	int -0.02 to 0.02	int 0.02 to 0.1	DFT E
B3LYP-D3	0.488	0.034	-1.231	0.884
PBE-D3	0.453	0.005	-1.800	0.868
M062X	0.520	0.038	0.494	0.957
PBE	1.759	-3.778	-3.207	0.947

Table 1.4: Coefficients of the linear regression. The corresponding scores are presented in Table 1.3

1.4 Hyperparametrization

The parameter γ was set to the inverse of the number of features, and c_0 to 1.0. The degree of the polynomial kernel and the value of α have been determined with a grid search. The following values have been considered:

- degree of polynomial: 1, 2, 3;
- α: 1.0. 0.1, 0.01.

Optimization of the degree of the polynomial for the B3LYP-D3 values yielded a value of 2, which has been maintained in all calculations. The value of α is 0.1 for B3LYP-D3 and PBE-D3. It assumes a value of 0.01 for PBE and of 1.0 for M062X.

1.5 Results for M06-2X, PBE-D3 and PBE functionals

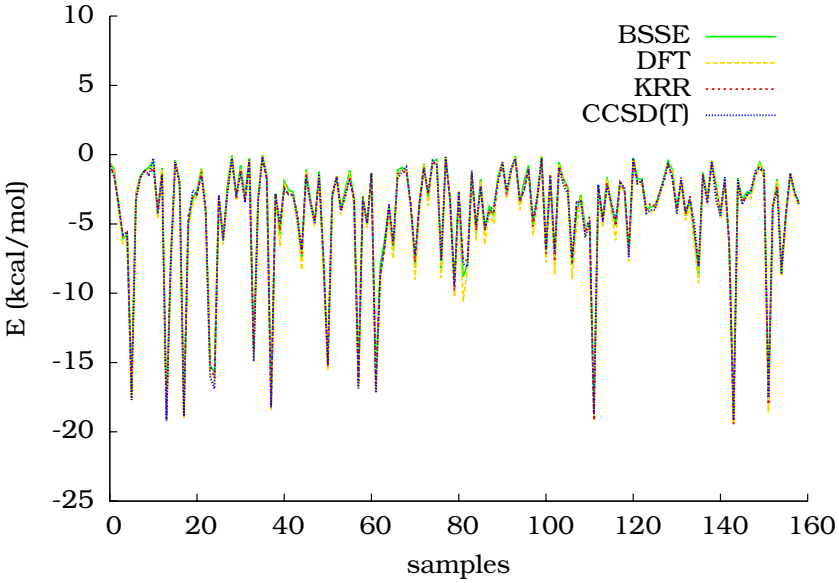

Figure 1.1: Interactions energies predicted at the DFT and BSSE-corrected DFT level and prediction using the KRR algorithm. Functional: M06-2X.

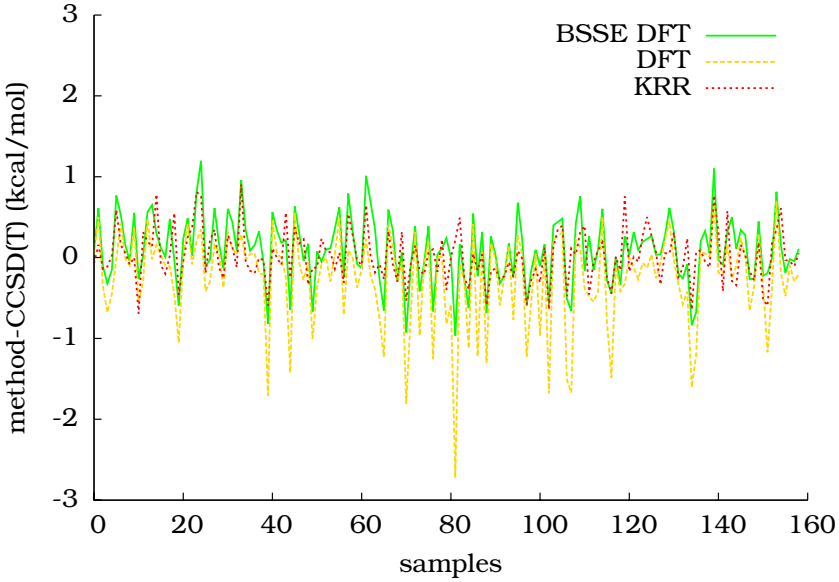

Figure 1.2: Error on the interactions energies predicted at the DFT and BSSE-corrected DFT level and prediction using the KRR algorithm. Functional: M06-2X.

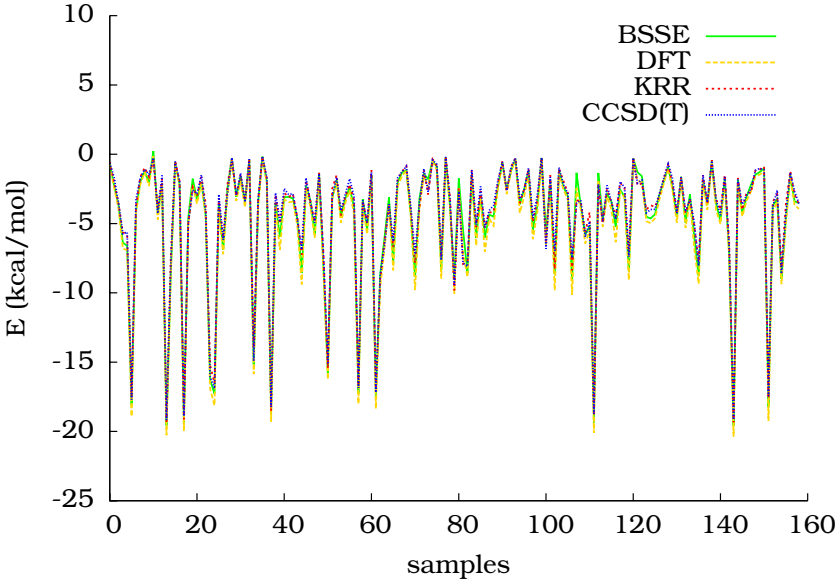

Figure 1.3: Interactions energies predicted at the DFT and BSSE-corrected DFT level and prediction using the KRR algorithm. Functional: PBE-D3.

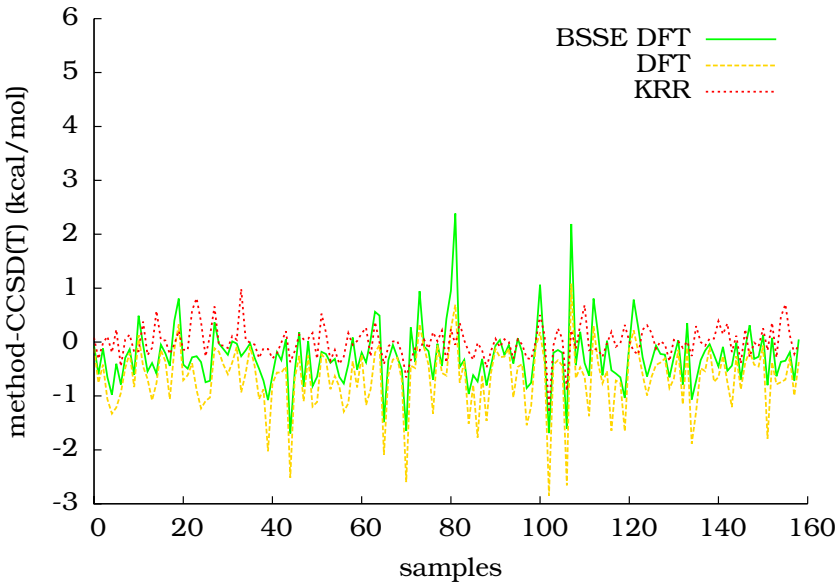

Figure 1.4: Error on the interactions energies predicted at the DFT and BSSE-corrected DFT level and prediction using the KRR algorithm. Functional: PBE-D3.

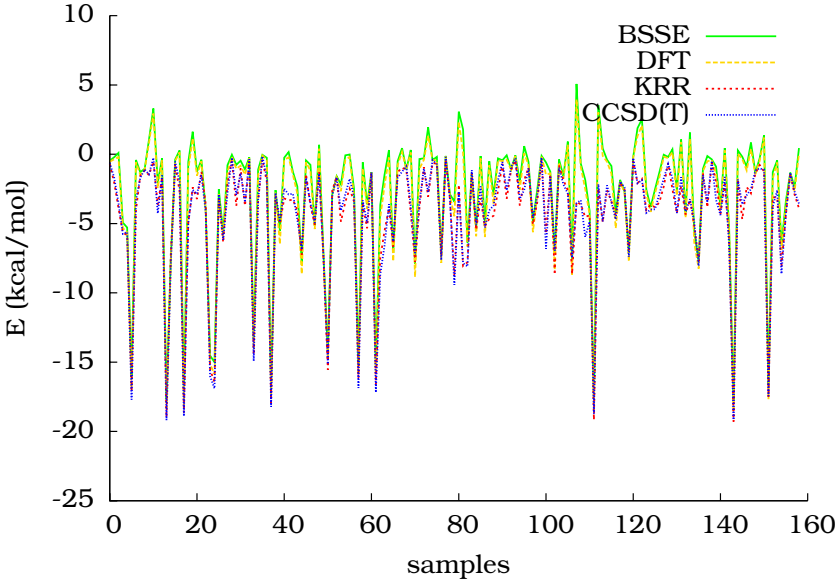

Figure 1.5: Interactions energies predicted at the DFT and BSSE-corrected DFT level and prediction using the KRR algorithm. Functional: PBE.

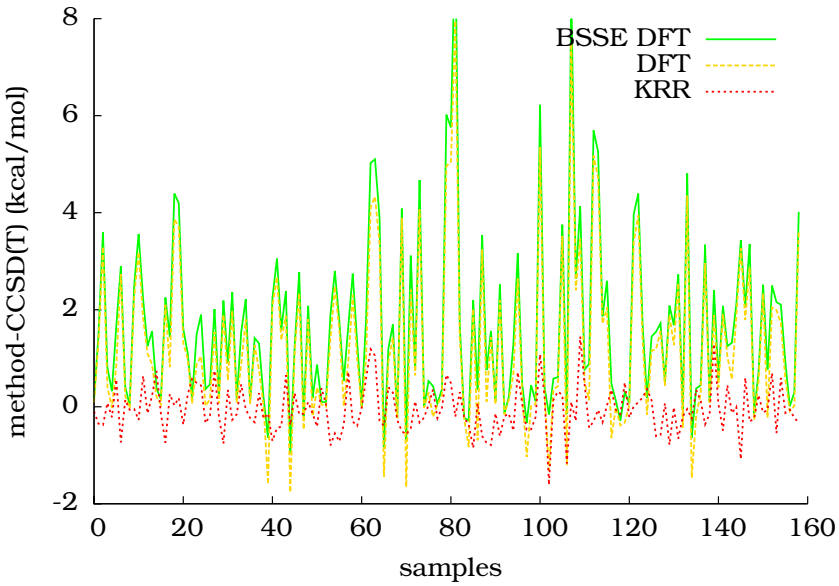

Figure 1.6: Error on the interactions energies predicted at the DFT and BSSE-corrected DFT level and prediction using the KRR algorithm. Functional: PBE.

name	-0.1 to -0.02	-0.02 to 0.02	0.02 to 0.1
01 Water-Water 0.90 nci	0.333	0.065	0.025
01 Water-Water 0.95 nci	0.253	0.071	0.004
01 Water-Water 1.00 nci	0.150	0.073	0.000
01 Water-Water 1.05 nci	0.098	0.078	0.000
01 Water-Water 1.10 nci	0.031	0.075	0.000
01 Water-Water 1.25 nci	0.000	0.037	0.000
01 Water-Water 1.50 nci	0.000	0.008	0.000
01 Water-Water 2.00 nci	0.000	0.001	0.000
02 Water-MeOH 0.90 nci	0.372	0.151	0.110
02 Water-MeOH 0.95 nci	0.303	0.149	0.062
02 Water-MeOH 1.00 nci	0.235	0.146	0.027
02 Water-MeOH 1.05 nci	0.150	0.144	0.017
02 Water-MeOH 1.10 nci	0.088	0.137	0.004
02 Water-MeOH 1.25 nci	0.004	0.070	0.000
02 Water-MeOH 1.50 nci	0.000	0.017	0.000
02 Water-MeOH 2.00 nci	0.000	0.001	0.000
03 Water-MeNH2 0.90 nci	0.491	0.127	0.088
03 Water-MeNH2 0.95 nci	0.412	0.122	0.041
03 Water-MeNH2 1.00 nci	0.328	0.115	0.009
03 Water-MeNH2 1.05 nci	0.232	0.111	0.000
03 Water-MeNH2 1.10 nci	0.148	0.113	0.000
03 Water-MeNH2 1.25 nci	0.010	0.078	0.000
03 Water-MeNH2 1.50 nci	0.000	0.018	0.000
03 Water-MeNH2 2.00 nci	0.000	0.001	0.000
04 Water-Peptide 0.90 nci	0.415	0.229	0.211
04 Water-Peptide 0.95 nci	0.356	0.237	0.140
04 Water-Peptide 1.00 nci	0.284	0.237	0.089
04 Water-Peptide 1.05 nci	0.217	0.238	0.050
04 Water-Peptide 1.10 nci	0.143	0.237	0.032
04 Water-Peptide 1.25 nci	0.015	0.183	0.000
04 Water-Peptide 1.50 nci	0.000	0.056	0.000
04 Water-Peptide 2.00 nci	0.000	0.005	0.000
05 MeOH-MeOH 0.90 nci	0.395	0.172	0.105
05 MeOH-MeOH 0.95 nci	0.337	0.156	0.053
05 MeOH-MeOH 1.00 nci	0.255	0.146	0.024
05 MeOH-MeOH 1.05 nci	0.180	0.141	0.009
05 MeOH-MeOH 1.10 nci	0.105	0.133	0.006
05 MeOH-MeOH 1.25 nci	0.008	0.075	0.000
05 MeOH-MeOH 1.50 nci	0.000	0.020	0.000
05 MeOH-MeOH 2.00 nci	0.000	0.002	0.000
06 MeOH-MeNH2 0.90 nci	0.490	0.343	0.181
06 MeOH-MeNH2 0.95 nci	0.441	0.304	0.100
06 MeOH-MeNH2 1.00 nci	0.353	0.276	0.044
06 MeOH-MeNH2 1.05 nci	0.286	0.245	0.015

Table 1.5: Electron density integrals obtained from the promolecular density - I.

name	-0.1 to -0.02	-0.02 to 0.02	0.02 to 0.1
06 MeOH-MeNH2 1.10 nci	0.190	0.220	0.004
06 MeOH-MeNH2 1.25 nci	0.029	0.125	0.000
06 MeOH-MeNH2 1.50 nci	0.000	0.032	0.000
06 MeOH-MeNH2 2.00 nci	0.000	0.002	0.000
07 MeOH-Peptide 0.90 nci	0.459	0.313	0.204
07 MeOH-Peptide 0.95 nci	0.404	0.301	0.132
07 MeOH-Peptide 1.00 nci	0.334	0.292	0.078
07 MeOH-Peptide 1.05 nci	0.263	0.281	0.041
07 MeOH-Peptide 1.10 nci	0.184	0.264	0.021
07 MeOH-Peptide 1.25 nci	0.024	0.195	0.001
07 MeOH-Peptide 1.50 nci	0.000	0.054	0.000
07 MeOH-Peptide 2.00 nci	0.000	0.002	0.000
08 MeOH-Water 0.90 nci	0.350	0.071	0.032
08 MeOH-Water 0.95 nci	0.255	0.073	0.009
08 MeOH-Water 1.00 nci	0.189	0.074	0.000
08 MeOH-Water 1.05 nci	0.109	0.077	0.000
08 MeOH-Water 1.10 nci	0.042	0.079	0.000
08 MeOH-Water 1.25 nci	0.001	0.042	0.000
08 MeOH-Water 1.50 nci	0.000	0.009	0.000
08 MeOH-Water 2.00 nci	0.000	0.001	0.000
09 MeNH2-MeOH 0.90 nci	0.200	0.303	0.020
09 MeNH2-MeOH 0.95 nci	0.110	0.259	0.004
09 MeNH2-MeOH 1.00 nci	0.039	0.202	0.002
09 MeNH2-MeOH 1.05 nci	0.015	0.147	0.000
09 MeNH2-MeOH 1.10 nci	0.002	0.104	0.000
09 MeNH2-MeOH 1.25 nci	0.000	0.042	0.000
09 MeNH2-MeOH 1.50 nci	0.000	0.010	0.000
09 MeNH2-MeOH 2.00 nci	0.000	0.001	0.000
10 MeNH2-MeNH2 0.90 nci	0.399	0.403	0.187
10 MeNH2-MeNH2 0.95 nci	0.287	0.389	0.103
10 MeNH2-MeNH2 1.00 nci	0.189	0.368	0.057
10 MeNH2-MeNH2 1.05 nci	0.104	0.329	0.027
10 MeNH2-MeNH2 1.10 nci	0.055	0.279	0.011
10 MeNH2-MeNH2 1.25 nci	0.000	0.111	0.000
10 MeNH2-MeNH2 1.50 nci	0.000	0.016	0.000
10 MeNH2-MeNH2 2.00 nci	0.000	0.001	0.000
11 MeNH2-Peptide 0.90 nci	0.378	0.505	0.189
11 MeNH2-Peptide 0.95 nci	0.262	0.492	0.117
11 MeNH2-Peptide 1.00 nci	0.160	0.471	0.069
11 MeNH2-Peptide 1.05 nci	0.088	0.428	0.035
11 MeNH2-Peptide 1.10 nci	0.044	0.372	0.016
11 MeNH2-Peptide 1.25 nci	0.000	0.109	0.000
11 MeNH2-Peptide 1.50 nci	0.000	0.017	0.000
11 MeNH2-Peptide 2.00 nci	0.000	0.001	0.000

Table 1.6: Electron density integrals obtained from the promolecular density - II.

name	-0.1 to -0.02	-0.02 to 0.02	0.02 to 0.1
12 MeNH2-Water 0.90 nci	0.503	0.162	0.213
12 MeNH2-Water 0.95 nci	0.440	0.166	0.138
12 MeNH2-Water 1.00 nci	0.369	0.166	0.085
12 MeNH2-Water 1.05 nci	0.297	0.168	0.049
12 MeNH2-Water 1.10 nci	0.209	0.166	0.033
12 MeNH2-Water 1.25 nci	0.038	0.137	0.007
12 MeNH2-Water 1.50 nci	0.000	0.034	0.000
12 MeNH2-Water 2.00 nci	0.000	0.003	0.000
13 Peptide-MeOH 0.90 nci	0.362	0.345	0.112
13 Peptide-MeOH 0.95 nci	0.278	0.318	0.052
13 Peptide-MeOH 1.00 nci	0.206	0.288	0.021
13 Peptide-MeOH 1.05 nci	0.121	0.263	0.006
13 Peptide-MeOH 1.10 nci	0.058	0.227	0.003
13 Peptide-MeOH 1.25 nci	0.001	0.108	0.000
13 Peptide-MeOH 1.50 nci	0.000	0.029	0.000
13 Peptide-MeOH 2.00 nci	0.000	0.003	0.000
14 Peptide-MeNH2 0.90 nci	0.489	0.460	0.189
14 Peptide-MeNH2 0.95 nci	0.400	0.419	0.099
14 Peptide-MeNH2 1.00 nci	0.314	0.379	0.044
14 Peptide-MeNH2 1.05 nci	0.218	0.341	0.017
14 Peptide-MeNH2 1.10 nci	0.139	0.304	0.010
14 Peptide-MeNH2 1.25 nci	0.009	0.156	0.000
14 Peptide-MeNH2 1.50 nci	0.000	0.038	0.000
14 Peptide-MeNH2 2.00 nci	0.000	0.003	0.000
15 Peptide-Peptide 0.90 nci	0.414	0.561	0.155
15 Peptide-Peptide 0.95 nci	0.326	0.523	0.086
15 Peptide-Peptide 1.00 nci	0.246	0.478	0.036
15 Peptide-Peptide 1.05 nci	0.173	0.433	0.015
15 Peptide-Peptide 1.10 nci	0.090	0.381	0.005
15 Peptide-Peptide 1.25 nci	0.005	0.210	0.000
15 Peptide-Peptide 1.50 nci	0.000	0.062	0.000
15 Peptide-Peptide 2.00 nci	0.000	0.005	0.000
16 Peptide-Water 0.90 nci	0.296	0.121	0.013
16 Peptide-Water 0.95 nci	0.192	0.116	0.000
16 Peptide-Water 1.00 nci	0.124	0.113	0.000
16 Peptide-Water 1.05 nci	0.043	0.109	0.000
16 Peptide-Water 1.10 nci	0.017	0.092	0.000
16 Peptide-Water 1.25 nci	0.000	0.037	0.000
16 Peptide-Water 1.50 nci	0.000	0.009	0.000
16 Peptide-Water 2.00 nci	0.000	0.000	0.000
17 Uracil-Uracil BP 0.90 nci	0.843	0.232	0.337
17 Uracil-Uracil BP 0.95 nci	0.745	0.247	0.214
17 Uracil-Uracil BP 1.00 nci	0.633	0.254	0.125
17 Uracil-Uracil BP 1.05 nci	0.506	0.263	0.057

Table 1.7: Electron density integrals obtained from the promolecular density - III.

name	-0.1 to -0.02	-0.02 to 0.02	0.02 to 0.1
17 Uracil-Uracil BP 1.10 nci	0.408	0.263	0.020
17 Uracil-Uracil BP 1.25 nci	0.052	0.229	0.000
17 Uracil-Uracil BP 1.50 nci	0.000	0.070	0.000
17 Uracil-Uracil BP 2.00 nci	0.000	0.008	0.000
18 Water-Pyridine 0.90 nci	0.477	0.142	0.098
18 Water-Pyridine 0.95 nci	0.405	0.138	0.056
18 Water-Pyridine 1.00 nci	0.325	0.133	0.019
18 Water-Pyridine 1.05 nci	0.248	0.123	0.004
18 Water-Pyridine 1.10 nci	0.157	0.115	0.000
18 Water-Pyridine 1.25 nci	0.013	0.080	0.000
18 Water-Pyridine 1.50 nci	0.000	0.019	0.000
18 Water-Pyridine 2.00 nci	0.000	0.001	0.000
19 MeOH-Pyridine 0.90 nci	0.492	0.228	0.158
19 MeOH-Pyridine 0.95 nci	0.432	0.206	0.093
19 MeOH-Pyridine 1.00 nci	0.363	0.188	0.040
19 MeOH-Pyridine 1.05 nci	0.294	0.166	0.009
19 MeOH-Pyridine 1.10 nci	0.200	0.140	0.001
19 MeOH-Pyridine 1.25 nci	0.031	0.099	0.000
19 MeOH-Pyridine 1.50 nci	0.000	0.025	0.000
19 MeOH-Pyridine 2.00 nci	0.000	0.002	0.000
20 AcOH-AcOH 0.90 nci	0.897	0.183	0.466
20 AcOH-AcOH 0.95 nci	0.858	0.200	0.330
20 AcOH-AcOH 1.00 nci	0.778	0.216	0.226
20 AcOH-AcOH 1.05 nci	0.673	0.228	0.138
20 AcOH-AcOH 1.10 nci	0.554	0.239	0.078
20 AcOH-AcOH 1.25 nci	0.188	0.255	0.007
20 AcOH-AcOH 1.50 nci	0.000	0.110	0.000
20 AcOH-AcOH 2.00 nci	0.000	0.011	0.000
21 AcNH2-AcNH2 0.90 nci	0.810	0.237	0.326
21 AcNH2-AcNH2 0.95 nci	0.706	0.253	0.209
21 AcNH2-AcNH2 1.00 nci	0.595	0.266	0.118
21 AcNH2-AcNH2 1.05 nci	0.473	0.274	0.057
21 AcNH2-AcNH2 1.10 nci	0.315	0.282	0.028
21 AcNH2-AcNH2 1.25 nci	0.029	0.228	0.002
21 AcNH2-AcNH2 1.50 nci	0.000	0.062	0.000
21 AcNH2-AcNH2 2.00 nci	0.000	0.005	0.000
22 AcOH-Uracil 0.90 nci	0.867	0.210	0.425
22 AcOH-Uracil 0.95 nci	0.802	0.227	0.279
22 AcOH-Uracil 1.00 nci	0.735	0.235	0.185
22 AcOH-Uracil 1.05 nci	0.629	0.248	0.110
22 AcOH-Uracil 1.10 nci	0.499	0.256	0.049
22 AcOH-Uracil 1.25 nci	0.121	0.257	0.004
22 AcOH-Uracil 1.50 nci	0.000	0.093	0.000
22 AcOH-Uracil 2.00 nci	0.000	0.010	0.000

Table 1.8: Electron density integrals obtained from the promolecular density - IV.

name	-0.1 to -0.02	-0.02 to 0.02	0.02 to 0.1
23 AcNH2-Uracil 0.90 nci	0.824	0.236	0.380
23 AcNH2-Uracil 0.95 nci	0.729	0.250	0.251
23 AcNH2-Uracil 1.00 nci	0.645	0.261	0.159
23 AcNH2-Uracil 1.05 nci	0.525	0.270	0.089
23 AcNH2-Uracil 1.10 nci	0.400	0.274	0.050
23 AcNH2-Uracil 1.25 nci	0.075	0.253	0.005
23 AcNH2-Uracil 1.50 nci	0.000	0.084	0.000
23 AcNH2-Uracil 2.00 nci	0.000	0.010	0.000
24 Benzene-Benzene pi-pi 0.90 nci	0.373	1.275	0.469
24 Benzene-Benzene pi-pi 0.95 nci	0.153	1.167	0.181
24 Benzene-Benzene pi-pi 1.00 nci	0.044	0.947	0.047
24 Benzene-Benzene pi-pi 1.05 nci	0.007	0.662	0.004
24 Benzene-Benzene pi-pi 1.10 nci	0.000	0.399	0.000
24 Benzene-Benzene pi-pi 1.25 nci	0.000	0.082	0.000
24 Benzene-Benzene pi-pi 1.50 nci	0.000	0.009	0.000
24 Benzene-Benzene pi-pi 2.00 nci	0.000	0.000	0.000
25 Pyridine-Pyridine pi-pi 0.90 nci	0.448	1.211	0.529
25 Pyridine-Pyridine pi-pi 0.95 nci	0.207	1.143	0.239
25 Pyridine-Pyridine pi-pi 1.00 nci	0.077	0.969	0.080
25 Pyridine-Pyridine pi-pi 1.05 nci	0.020	0.719	0.018
25 Pyridine-Pyridine pi-pi 1.10 nci	0.002	0.464	0.001
25 Pyridine-Pyridine pi-pi 1.25 nci	0.000	0.106	0.000
25 Pyridine-Pyridine pi-pi 1.50 nci	0.000	0.013	0.000
25 Pyridine-Pyridine pi-pi 2.00 nci	0.000	0.000	0.000
26 Uracil-Uracil pi-pi 0.90 nci	0.585	1.173	0.722
26 Uracil-Uracil pi-pi 0.95 nci	0.302	1.198	0.371
26 Uracil-Uracil pi-pi 1.00 nci	0.150	1.073	0.157
26 Uracil-Uracil pi-pi 1.05 nci	0.061	0.872	0.048
26 Uracil-Uracil pi-pi 1.10 nci	0.008	0.593	0.006
26 Uracil-Uracil pi-pi 1.25 nci	0.000	0.162	0.000
26 Uracil-Uracil pi-pi 1.50 nci	0.000	0.031	0.000
26 Uracil-Uracil pi-pi 2.00 nci	0.000	0.001	0.000
27 Benzene-Pyridine pi-pi 0.90 nci	0.454	1.230	0.543
27 Benzene-Pyridine pi-pi 0.95 nci	0.195	1.156	0.223
27 Benzene-Pyridine pi-pi 1.00 nci	0.064	0.961	0.059
27 Benzene-Pyridine pi-pi 1.05 nci	0.012	0.695	0.005
27 Benzene-Pyridine pi-pi 1.10 nci	0.000	0.427	0.000
27 Benzene-Pyridine pi-pi 1.25 nci	0.000	0.093	0.000
27 Benzene-Pyridine pi-pi 1.50 nci	0.000	0.011	0.000
27 Benzene-Pyridine pi-pi 2.00 nci	0.000	0.000	0.000
28 Benzene-Uracil pi-pi 0.90 nci	0.499	1.240	0.632
28 Benzene-Uracil pi-pi 0.95 nci	0.258	1.212	0.295
28 Benzene-Uracil pi-pi 1.00 nci	0.108	1.063	0.102
28 Benzene-Uracil pi-pi 1.05 nci	0.019	0.826	0.015

Table 1.9: Electron density integrals obtained from the promolecular density - V.

name	-0.1 to -0.02	-0.02 to 0.02	0.02 to 0.1
28 Benzene-Uracil pi-pi 1.10 nci	0.001	0.541	0.000
28 Benzene-Uracil pi-pi 1.25 nci	0.000	0.130	0.000
28 Benzene-Uracil pi-pi 1.50 nci	0.000	0.020	0.000
28 Benzene-Uracil pi-pi 2.00 nci	0.000	0.001	0.000
29 Pyridine-Uracil pi-pi 0.90 nci	0.623	1.125	0.744
29 Pyridine-Uracil pi-pi 0.95 nci	0.288	1.147	0.331
29 Pyridine-Uracil pi-pi 1.00 nci	0.104	0.999	0.097
29 Pyridine-Uracil pi-pi 1.05 nci	0.022	0.737	0.012
29 Pyridine-Uracil pi-pi 1.10 nci	0.000	0.441	0.000
29 Pyridine-Uracil pi-pi 1.25 nci	0.000	0.099	0.000
29 Pyridine-Uracil pi-pi 1.50 nci	0.000	0.013	0.000
29 Pyridine-Uracil pi-pi 2.00 nci	0.000	0.000	0.000
30 Benzene-Ethene 0.90 nci	0.216	0.836	0.210
30 Benzene-Ethene 0.95 nci	0.078	0.717	0.077
30 Benzene-Ethene 1.00 nci	0.009	0.560	0.009
30 Benzene-Ethene 1.05 nci	0.000	0.331	0.000
30 Benzene-Ethene 1.10 nci	0.000	0.190	0.000
30 Benzene-Ethene 1.25 nci	0.000	0.046	0.000
30 Benzene-Ethene 1.50 nci	0.000	0.006	0.000
30 Benzene-Ethene 2.00 nci	0.000	0.000	0.000
31 Uracil-Ethene 0.90 nci	0.257	0.776	0.266
31 Uracil-Ethene 0.95 nci	0.113	0.712	0.123
31 Uracil-Ethene 1.00 nci	0.035	0.596	0.037
31 Uracil-Ethene 1.05 nci	0.008	0.432	0.005
31 Uracil-Ethene 1.10 nci	0.000	0.251	0.000
31 Uracil-Ethene 1.25 nci	0.000	0.069	0.000
31 Uracil-Ethene 1.50 nci	0.000	0.011	0.000
31 Uracil-Ethene 2.00 nci	0.000	0.000	0.000
32 Uracil-Ethyne 0.90 nci	0.277	0.651	0.247
32 Uracil-Ethyne 0.95 nci	0.124	0.607	0.119
32 Uracil-Ethyne 1.00 nci	0.048	0.503	0.043
32 Uracil-Ethyne 1.05 nci	0.016	0.370	0.009
32 Uracil-Ethyne 1.10 nci	0.002	0.235	0.000
32 Uracil-Ethyne 1.25 nci	0.000	0.063	0.000
32 Uracil-Ethyne 1.50 nci	0.000	0.010	0.000
32 Uracil-Ethyne 2.00 nci	0.000	0.000	0.000
33 Pyridine-Ethene 0.90 nci	0.236	0.798	0.211
33 Pyridine-Ethene 0.95 nci	0.096	0.709	0.088
33 Pyridine-Ethene 1.00 nci	0.017	0.565	0.020
33 Pyridine-Ethene 1.05 nci	0.001	0.382	0.000
33 Pyridine-Ethene 1.10 nci	0.000	0.209	0.000
33 Pyridine-Ethene 1.25 nci	0.000	0.058	0.000
33 Pyridine-Ethene 1.50 nci	0.000	0.009	0.000
33 Pyridine-Ethene 2.00 nci	0.000	0.000	0.000

Table 1.10: Electron density integrals obtained from the promolecular density - VI.

name	-0.1 to -0.02	-0.02 to 0.02	0.02 to 0.1
34 Pentane-Pentane 0.90 nci	0.622	1.785	0.452
34 Pentane-Pentane 0.95 nci	0.329	1.679	0.177
34 Pentane-Pentane 1.00 nci	0.132	1.472	0.043
34 Pentane-Pentane 1.05 nci	0.027	1.162	0.006
34 Pentane-Pentane 1.10 nci	0.001	0.818	0.000
34 Pentane-Pentane 1.25 nci	0.000	0.238	0.000
34 Pentane-Pentane 1.50 nci	0.000	0.047	0.000
34 Pentane-Pentane 2.00 nci	0.000	0.003	0.000
35 Neopentane-Pentane 0.90 nci	0.473	1.232	0.235
35 Neopentane-Pentane 0.95 nci	0.216	1.089	0.097
35 Neopentane-Pentane 1.00 nci	0.070	0.888	0.025
35 Neopentane-Pentane 1.05 nci	0.007	0.642	0.002
35 Neopentane-Pentane 1.10 nci	0.000	0.437	0.000
35 Neopentane-Pentane 1.25 nci	0.000	0.125	0.000
35 Neopentane-Pentane 1.50 nci	0.000	0.024	0.000
35 Neopentane-Pentane 2.00 nci	0.000	0.001	0.000
36 Neopentane-Neopentane 0.90 nci	0.206	0.944	0.001
36 Neopentane-Neopentane 0.95 nci	0.061	0.753	0.000
36 Neopentane-Neopentane 1.00 nci	0.000	0.499	0.000
36 Neopentane-Neopentane 1.05 nci	0.000	0.341	0.000
36 Neopentane-Neopentane 1.10 nci	0.000	0.239	0.000
36 Neopentane-Neopentane 1.25 nci	0.000	0.074	0.000
36 Neopentane-Neopentane 1.50 nci	0.000	0.015	0.000
36 Neopentane-Neopentane 2.00 nci	0.000	0.001	0.000
37 Cyclopentane-Neopentane 0.90 nci	0.515	1.229	0.208
37 Cyclopentane-Neopentane 0.95 nci	0.263	1.116	0.065
37 Cyclopentane-Neopentane 1.00 nci	0.105	0.935	0.010
37 Cyclopentane-Neopentane 1.05 nci	0.013	0.684	0.001
37 Cyclopentane-Neopentane 1.10 nci	0.000	0.460	0.000
37 Cyclopentane-Neopentane 1.25 nci	0.000	0.144	0.000
37 Cyclopentane-Neopentane 1.50 nci	0.000	0.028	0.000
37 Cyclopentane-Neopentane 2.00 nci	0.000	0.002	0.000
38 Cyclopentane-Cyclopentane 0.90 nci	0.556	1.350	0.260
38 Cyclopentane-Cyclopentane 0.95 nci	0.309	1.274	0.101
38 Cyclopentane-Cyclopentane 1.00 nci	0.131	1.101	0.020
38 Cyclopentane-Cyclopentane 1.05 nci	0.019	0.851	0.001
38 Cyclopentane-Cyclopentane 1.10 nci	0.000	0.565	0.000
38 Cyclopentane-Cyclopentane 1.25 nci	0.000	0.156	0.000
38 Cyclopentane-Cyclopentane 1.50 nci	0.000	0.032	0.000
38 Cyclopentane-Cyclopentane 2.00 nci	0.000	0.002	0.000
39 Benzene-Cyclopentane 0.90 nci	0.516	1.224	0.479
39 Benzene-Cyclopentane 0.95 nci	0.272	1.177	0.236
39 Benzene-Cyclopentane 1.00 nci	0.109	1.011	0.095
39 Benzene-Cyclopentane 1.05 nci	0.028	0.803	0.019

Table 1.11: Electron density integrals obtained from the promolecular density - VII.

name	-0.1 to -0.02	-0.02 to 0.02	0.02 to 0.1
39 Benzene-Cyclopentane 1.10 nci	0.002	0.534	0.000
39 Benzene-Cyclopentane 1.25 nci	0.000	0.139	0.000
39 Benzene-Cyclopentane 1.50 nci	0.000	0.023	0.000
39 Benzene-Cyclopentane 2.00 nci	0.000	0.000	0.000
40 Benzene-Neopentane 0.90 nci	0.360	1.005	0.291
40 Benzene-Neopentane 0.95 nci	0.158	0.885	0.151
40 Benzene-Neopentane 1.00 nci	0.051	0.711	0.060
40 Benzene-Neopentane 1.05 nci	0.006	0.519	0.007
40 Benzene-Neopentane 1.10 nci	0.000	0.330	0.000
40 Benzene-Neopentane 1.25 nci	0.000	0.088	0.000
40 Benzene-Neopentane 1.50 nci	0.000	0.014	0.000
40 Benzene-Neopentane 2.00 nci	0.000	0.000	0.000
41 Uracil-Pentane 0.90 nci	0.469	1.412	0.530
41 Uracil-Pentane 0.95 nci	0.232	1.318	0.262
41 Uracil-Pentane 1.00 nci	0.080	1.126	0.110
41 Uracil-Pentane 1.05 nci	0.019	0.862	0.027
41 Uracil-Pentane 1.10 nci	0.000	0.542	0.000
41 Uracil-Pentane 1.25 nci	0.000	0.129	0.000
41 Uracil-Pentane 1.50 nci	0.000	0.020	0.000
41 Uracil-Pentane 2.00 nci	0.000	0.000	0.000
42 Uracil-Cyclopentane 0.90 nci	0.452	1.199	0.463
42 Uracil-Cyclopentane 0.95 nci	0.216	1.125	0.228
42 Uracil-Cyclopentane 1.00 nci	0.064	0.967	0.091
42 Uracil-Cyclopentane 1.05 nci	0.012	0.724	0.016
42 Uracil-Cyclopentane 1.10 nci	0.000	0.473	0.000
42 Uracil-Cyclopentane 1.25 nci	0.000	0.130	0.000
42 Uracil-Cyclopentane 1.50 nci	0.000	0.024	0.000
42 Uracil-Cyclopentane 2.00 nci	0.000	0.001	0.000
43 Uracil-Neopentane 0.90 nci	0.326	0.992	0.361
43 Uracil-Neopentane 0.95 nci	0.149	0.900	0.172
43 Uracil-Neopentane 1.00 nci	0.042	0.745	0.054
43 Uracil-Neopentane 1.05 nci	0.005	0.535	0.007
43 Uracil-Neopentane 1.10 nci	0.000	0.338	0.000
43 Uracil-Neopentane 1.25 nci	0.000	0.096	0.000
43 Uracil-Neopentane 1.50 nci	0.000	0.017	0.000
43 Uracil-Neopentane 2.00 nci	0.000	0.001	0.000
44 Ethene-Pentane 0.90 nci	0.266	0.927	0.174
44 Ethene-Pentane 0.95 nci	0.131	0.820	0.059
44 Ethene-Pentane 1.00 nci	0.046	0.667	0.018
44 Ethene-Pentane 1.05 nci	0.008	0.496	0.002
44 Ethene-Pentane 1.10 nci	0.000	0.334	0.000
44 Ethene-Pentane 1.25 nci	0.000	0.095	0.000
44 Ethene-Pentane 1.50 nci	0.000	0.018	0.000
44 Ethene-Pentane 2.00 nci	0.000	0.001	0.000

Table 1.12: Electron density integrals obtained from the promolecular density - VIII.

name	-0.1 to -0.02	-0.02 to 0.02	0.02 to 0.1
45 Ethyne-Pentane 0.90 nci	0.221	0.822	0.081
45 Ethyne-Pentane 0.95 nci	0.091	0.682	0.022
45 Ethyne-Pentane 1.00 nci	0.026	0.505	0.005
45 Ethyne-Pentane 1.05 nci	0.001	0.325	0.000
45 Ethyne-Pentane 1.10 nci	0.000	0.204	0.000
45 Ethyne-Pentane 1.25 nci	0.000	0.055	0.000
45 Ethyne-Pentane 1.50 nci	0.000	0.009	0.000
45 Ethyne-Pentane 2.00 nci	0.000	0.000	0.000
46 Peptide-Pentane 0.90 nci	0.382	1.392	0.362
46 Peptide-Pentane 0.95 nci	0.193	1.301	0.179
46 Peptide-Pentane 1.00 nci	0.084	1.136	0.077
46 Peptide-Pentane 1.05 nci	0.023	0.923	0.020
46 Peptide-Pentane 1.10 nci	0.001	0.678	0.001
46 Peptide-Pentane 1.25 nci	0.000	0.212	0.000
46 Peptide-Pentane 1.50 nci	0.000	0.039	0.000
46 Peptide-Pentane 2.00 nci	0.000	0.002	0.000
47 Benzene-Benzene TS 0.90 nci	0.447	0.623	0.425
47 Benzene-Benzene TS 0.95 nci	0.226	0.638	0.241
47 Benzene-Benzene TS 1.00 nci	0.109	0.567	0.126
47 Benzene-Benzene TS 1.05 nci	0.039	0.467	0.055
47 Benzene-Benzene TS 1.10 nci	0.006	0.364	0.010
47 Benzene-Benzene TS 1.25 nci	0.000	0.097	0.000
47 Benzene-Benzene TS 1.50 nci	0.000	0.015	0.000
47 Benzene-Benzene TS 2.00 nci	0.000	0.000	0.000
48 Pyridine-Pyridine TS 0.90 nci	0.393	0.621	0.379
48 Pyridine-Pyridine TS 0.95 nci	0.213	0.628	0.206
48 Pyridine-Pyridine TS 1.00 nci	0.100	0.576	0.097
48 Pyridine-Pyridine TS 1.05 nci	0.029	0.487	0.039
48 Pyridine-Pyridine TS 1.10 nci	0.005	0.371	0.003
48 Pyridine-Pyridine TS 1.25 nci	0.000	0.107	0.000
48 Pyridine-Pyridine TS 1.50 nci	0.000	0.020	0.000
48 Pyridine-Pyridine TS 2.00 nci	0.000	0.001	0.000
49 Benzene-Pyridine TS 0.90 nci	0.480	0.619	0.444
49 Benzene-Pyridine TS 0.95 nci	0.247	0.639	0.259
49 Benzene-Pyridine TS 1.00 nci	0.123	0.581	0.132
49 Benzene-Pyridine TS 1.05 nci	0.049	0.486	0.055
49 Benzene-Pyridine TS 1.10 nci	0.011	0.379	0.008
49 Benzene-Pyridine TS 1.25 nci	0.000	0.106	0.000
49 Benzene-Pyridine TS 1.50 nci	0.000	0.016	0.000
49 Benzene-Pyridine TS 2.00 nci	0.000	0.000	0.000
50 Benzene-Ethyne CH-pi 0.90 nci	0.480	0.373	0.363
50 Benzene-Ethyne CH-pi 0.95 nci	0.252	0.415	0.240
50 Benzene-Ethyne CH-pi 1.00 nci	0.123	0.403	0.137
50 Benzene-Ethyne CH-pi 1.05 nci	0.048	0.355	0.066

Table 1.13: Electron density integrals obtained from the promolecular density - IX.

name	-0.1 to -0.02	-0.02 to 0.02	0.02 to 0.1
50 Benzene-Ethyne CH-pi 1.10 nci	0.013	0.288	0.016
50 Benzene-Ethyne CH-pi 1.25 nci	0.000	0.086	0.000
50 Benzene-Ethyne CH-pi 1.50 nci	0.000	0.012	0.000
50 Benzene-Ethyne CH-pi 2.00 nci	0.000	0.000	0.000
51 Ethyne-Ethyne TS 0.90 nci	0.182	0.217	0.033
51 Ethyne-Ethyne TS 0.95 nci	0.092	0.196	0.019
51 Ethyne-Ethyne TS 1.00 nci	0.037	0.160	0.009
51 Ethyne-Ethyne TS 1.05 nci	0.010	0.118	0.003
51 Ethyne-Ethyne TS 1.10 nci	0.001	0.076	0.002
51 Ethyne-Ethyne TS 1.25 nci	0.000	0.023	0.000
51 Ethyne-Ethyne TS 1.50 nci	0.000	0.004	0.000
51 Ethyne-Ethyne TS 2.00 nci	0.000	0.000	0.000
52 Benzene-AcOH OH-pi 0.90 nci	0.512	0.386	0.402
52 Benzene-AcOH OH-pi 0.95 nci	0.372	0.385	0.274
52 Benzene-AcOH OH-pi 1.00 nci	0.234	0.388	0.181
52 Benzene-AcOH OH-pi 1.05 nci	0.131	0.377	0.109
52 Benzene-AcOH OH-pi 1.10 nci	0.066	0.337	0.055
52 Benzene-AcOH OH-pi 1.25 nci	0.000	0.160	0.000
52 Benzene-AcOH OH-pi 1.50 nci	0.000	0.026	0.000
52 Benzene-AcOH OH-pi 2.00 nci	0.000	0.001	0.000
53 Benzene-AcNH2 NH-pi 0.90 nci	0.387	0.462	0.204
53 Benzene-AcNH2 NH-pi 0.95 nci	0.256	0.449	0.117
53 Benzene-AcNH2 NH-pi 1.00 nci	0.147	0.420	0.060
53 Benzene-AcNH2 NH-pi 1.05 nci	0.080	0.360	0.027
53 Benzene-AcNH2 NH-pi 1.10 nci	0.035	0.289	0.011
53 Benzene-AcNH2 NH-pi 1.25 nci	0.000	0.093	0.000
53 Benzene-AcNH2 NH-pi 1.50 nci	0.000	0.018	0.000
53 Benzene-AcNH2 NH-pi 2.00 nci	0.000	0.001	0.000
54 Benzene-Water OH-pi 0.90 nci	0.337	0.409	0.214
54 Benzene-Water OH-pi 0.95 nci	0.210	0.411	0.115
54 Benzene-Water OH-pi 1.00 nci	0.115	0.388	0.047
54 Benzene-Water OH-pi 1.05 nci	0.058	0.326	0.016
54 Benzene-Water OH-pi 1.10 nci	0.022	0.260	0.001
54 Benzene-Water OH-pi 1.25 nci	0.000	0.086	0.000
54 Benzene-Water OH-pi 1.50 nci	0.000	0.014	0.000
54 Benzene-Water OH-pi 2.00 nci	0.000	0.000	0.000
55 Benzene-MeOH OH-pi 0.90 nci	0.464	0.616	0.394
55 Benzene-MeOH OH-pi 0.95 nci	0.307	0.601	0.259
55 Benzene-MeOH OH-pi 1.00 nci	0.172	0.566	0.158
55 Benzene-MeOH OH-pi 1.05 nci	0.089	0.499	0.092
55 Benzene-MeOH OH-pi 1.10 nci	0.038	0.425	0.043
55 Benzene-MeOH OH-pi 1.25 nci	0.000	0.168	0.000
55 Benzene-MeOH OH-pi 1.50 nci	0.000	0.029	0.000
55 Benzene-MeOH OH-pi 2.00 nci	0.000	0.001	0.000

Table 1.14: Electron density integrals obtained from the promolecular density - X.

name	-0.1 to -0.02	-0.02 to 0.02	0.02 to 0.1
56 Benzene-MeNH2 NH-pi 0.90 nci	0.385	0.676	0.352
56 Benzene-MeNH2 NH-pi 0.95 nci	0.207	0.648	0.206
56 Benzene-MeNH2 NH-pi 1.00 nci	0.110	0.576	0.116
56 Benzene-MeNH2 NH-pi 1.05 nci	0.043	0.472	0.055
56 Benzene-MeNH2 NH-pi 1.10 nci	0.009	0.364	0.013
56 Benzene-MeNH2 NH-pi 1.25 nci	0.000	0.107	0.000
56 Benzene-MeNH2 NH-pi 1.50 nci	0.000	0.016	0.000
56 Benzene-MeNH2 NH-pi 2.00 nci	0.000	0.000	0.000
57 Benzene-Peptide NH-pi 0.90 nci	0.652	0.868	0.560
57 Benzene-Peptide NH-pi 0.95 nci	0.377	0.832	0.347
57 Benzene-Peptide NH-pi 1.00 nci	0.193	0.757	0.193
57 Benzene-Peptide NH-pi 1.05 nci	0.090	0.635	0.099
57 Benzene-Peptide NH-pi 1.10 nci	0.034	0.510	0.038
57 Benzene-Peptide NH-pi 1.25 nci	0.000	0.166	0.000
57 Benzene-Peptide NH-pi 1.50 nci	0.000	0.025	0.000
57 Benzene-Peptide NH-pi 2.00 nci	0.000	0.001	0.000
58 Pyridine-Pyridine CH-N 0.90 nci	0.509	0.259	0.257
58 Pyridine-Pyridine CH-N 0.95 nci	0.309	0.299	0.155
58 Pyridine-Pyridine CH-N 1.00 nci	0.125	0.311	0.067
58 Pyridine-Pyridine CH-N 1.05 nci	0.038	0.262	0.025
58 Pyridine-Pyridine CH-N 1.10 nci	0.006	0.185	0.006
58 Pyridine-Pyridine CH-N 1.25 nci	0.000	0.044	0.000
58 Pyridine-Pyridine CH-N 1.50 nci	0.000	0.007	0.000
58 Pyridine-Pyridine CH-N 2.00 nci	0.000	0.000	0.000
59 Ethyne-Water CH-O 0.90 nci	0.174	0.077	0.000
59 Ethyne-Water CH-O 0.95 nci	0.093	0.079	0.000
59 Ethyne-Water CH-O 1.00 nci	0.030	0.076	0.000
59 Ethyne-Water CH-O 1.05 nci	0.013	0.065	0.000
59 Ethyne-Water CH-O 1.10 nci	0.003	0.047	0.000
59 Ethyne-Water CH-O 1.25 nci	0.000	0.016	0.000
59 Ethyne-Water CH-O 1.50 nci	0.000	0.003	0.000
59 Ethyne-Water CH-O 2.00 nci	0.000	0.000	0.000
60 Ethyne-AcOH OH-pi 0.90 nci	0.543	0.309	0.177
60 Ethyne-AcOH OH-pi 0.95 nci	0.409	0.303	0.104
60 Ethyne-AcOH OH-pi 1.00 nci	0.285	0.291	0.059
60 Ethyne-AcOH OH-pi 1.05 nci	0.174	0.281	0.037
60 Ethyne-AcOH OH-pi 1.10 nci	0.103	0.251	0.019
60 Ethyne-AcOH OH-pi 1.25 nci	0.005	0.118	0.001
60 Ethyne-AcOH OH-pi 1.50 nci	0.000	0.022	0.000
60 Ethyne-AcOH OH-pi 2.00 nci	0.000	0.001	0.000
61 Pentane-AcOH 0.90 nci	0.182	0.971	0.147
61 Pentane-AcOH 0.95 nci	0.089	0.880	0.056
61 Pentane-AcOH 1.00 nci	0.029	0.746	0.010
61 Pentane-AcOH 1.05 nci	0.005	0.564	0.001

Table 1.15: Electron density integrals obtained from the promolecular density - XI.

name	-0.1 to -0.02	-0.02 to 0.02	0.02 to 0.1
61 Pentane-AcOH 1.10 nci	0.000	0.407	0.000
61 Pentane-AcOH 1.25 nci	0.000	0.144	0.000
61 Pentane-AcOH 1.50 nci	0.000	0.026	0.000
61 Pentane-AcOH 2.00 nci	0.000	0.001	0.000
62 Pentane-AcNH2 0.90 nci	0.248	1.096	0.200
62 Pentane-AcNH2 0.95 nci	0.112	0.982	0.076
62 Pentane-AcNH2 1.00 nci	0.035	0.821	0.013
62 Pentane-AcNH2 1.05 nci	0.004	0.611	0.000
62 Pentane-AcNH2 1.10 nci	0.000	0.415	0.000
62 Pentane-AcNH2 1.25 nci	0.000	0.135	0.000
62 Pentane-AcNH2 1.50 nci	0.000	0.030	0.000
62 Pentane-AcNH2 2.00 nci	0.000	0.002	0.000
63 Benzene-AcOH 0.90 nci	0.383	0.782	0.440
63 Benzene-AcOH 0.95 nci	0.198	0.763	0.234
63 Benzene-AcOH 1.00 nci	0.086	0.674	0.111
63 Benzene-AcOH 1.05 nci	0.031	0.549	0.038
63 Benzene-AcOH 1.10 nci	0.005	0.407	0.003
63 Benzene-AcOH 1.25 nci	0.000	0.106	0.000
63 Benzene-AcOH 1.50 nci	0.000	0.016	0.000
63 Benzene-AcOH 2.00 nci	0.000	0.000	0.000
64 Peptide-Ethene 0.90 nci	0.169	0.656	0.160
64 Peptide-Ethene 0.95 nci	0.073	0.597	0.078
64 Peptide-Ethene 1.00 nci	0.022	0.511	0.029
64 Peptide-Ethene 1.05 nci	0.005	0.389	0.005
64 Peptide-Ethene 1.10 nci	0.000	0.266	0.000
64 Peptide-Ethene 1.25 nci	0.000	0.088	0.000
64 Peptide-Ethene 1.50 nci	0.000	0.018	0.000
64 Peptide-Ethene 2.00 nci	0.000	0.000	0.000
65 Pyridine-Ethyne 0.90 nci	0.331	0.148	0.026
65 Pyridine-Ethyne 0.95 nci	0.243	0.138	0.005
65 Pyridine-Ethyne 1.00 nci	0.133	0.131	0.000
65 Pyridine-Ethyne 1.05 nci	0.058	0.122	0.000
65 Pyridine-Ethyne 1.10 nci	0.019	0.102	0.000
65 Pyridine-Ethyne 1.25 nci	0.000	0.037	0.000
65 Pyridine-Ethyne 1.50 nci	0.000	0.008	0.000
65 Pyridine-Ethyne 2.00 nci	0.000	0.000	0.000
66 MeNH2-Pyridine 0.90 nci	0.391	0.582	0.239
66 MeNH2-Pyridine 0.95 nci	0.267	0.553	0.140
66 MeNH2-Pyridine 1.00 nci	0.159	0.516	0.074
66 MeNH2-Pyridine 1.05 nci	0.080	0.453	0.034
66 MeNH2-Pyridine 1.10 nci	0.031	0.371	0.012
66 MeNH2-Pyridine 1.25 nci	0.000	0.134	0.000
66 MeNH2-Pyridine 1.50 nci	0.000	0.031	0.000
66 MeNH2-Pyridine 2.00 nci	0.000	0.002	0.000

Table 1.16: Electron density integrals obtained from the promolecular density - XII.