Table 1S: Calculated heavy atom distances in Mg-P.

Mg-P distance[a)]	PM5[b)]	PM3[b)]	HF/6-31G*	B3LYP/6-31G*	exp.[c)]
1-2	1.470	1.455	1.419	1.447	1.451
2-3	1.355	1.360	1.367	1.364	1.344
3-4	1.472	1.465	1.419	1.447	1.475
4-5	1.416	1.417	1.415	1.401	1.368
5-6	1.358	1.362	1.367	1.401	1.418
6-7	1.491	1.475	1.444	1.446	1.463
7-8	1.343	1.358	1.347	1.366	1.360
8-9	1.491	1.475	1.449	1.446	1.461
9-10	1.361	1.362	1.414	1.401	1.378
10-11	1.412	1.417	1.371	1.400	1.414
11-12	1.477	1.465	1.464	1.446	1.419
12-13	1.352	1.360	1.334	1.365	1.406
13-14	1.475	1.455	1.464	1.447	1.417
13-13^1	----	----	----	----	1.429
13^1-13^2	----	----	----	----	1.569
13^2-15	----	----	----	----	1.534
14-15	1.352	1.373	1.370	1.400	1.396
15-16	1.417	1.399	1.415	1.401	1.364
16-17	1.438	1.446	1.448	1.446	1.523
17-18	1.379	1.372	1.346	1.366	1.555
18-19	1.438	1.447	1.444	1.446	1.525
19-20	1.411	1.399	1.367	1.401	1.382
20-1	1.356	1.373	1.415	1.401	1.388
NA-1	1.425	1.446	1.352	1.373	1.377
NA-4	1.354	1.371	1.351	1.372	1.385
NB-6	1.399	1.395	1.376	1.372	1.361
NB-9	1.393	1.395	1.330	1.373	1.389
NC-11	1.354	1.371	1.358	1.373	1.403
NC-14	1.425	1.446	1.357	1.373	1.347
ND-16	1.382	1.389	1.331	1.373	1.388
ND-19	1.388	1.389	1.376	1.372	1.349
Mg-NA	2.061	1.887	2.056	2.066	2.063
Mg-NB	2.049	1.825	2.058	2.066	2.093
Mg-NC	2.061	1.887	2.049	2.063	2.022
Mg-ND	2.057	2.467	2.058	2.065	2.167
A,B,C,Mg	0.003	0.000	0.000	0.000	0.385
NA-NB	2.893	2.848	2.920	2.919	2.922
NA-NC	4.122	3.715	4.105	4.129	4.011
NA-ND	2.929	2.829	2.920	2.919	2.954
NB-NC	2.889	2.848	2.893	2.920	2.782
NB-ND	4.107	4.293	4.116	4.129	4.191
NC-ND	2.926	2.829	2.892	2.920	2.946

a) 1 is C1; NA is nitrogen in ring A; A,B,C,Mg is the distance between plane NA-NB-NC and the Mg-atom.
b) From ref. 40.
c) From ref. 84.

Table 2S: Calculated heavy atom distances in Mg-C.

Mg-C distance[a)]	PM5[b)]	PM3[b)]	HF/6-31G*	B3LYP/6-31G*	exp.[c)]
1-2	1.477	1.465	1.453	1.445	1.451
2-3	1.353	1.355	1.343	1.366	1.344
3-4	1.472	1.467	1.446	1.442	1.475
4-5	1.350	1.367	1.353	1.391	1.368
5-6	1.417	1.406	1.430	1.408	1.418
6-7	1.434	1.436	1.403	1.438	1.463
7-8	1.382	1.384	1.380	1.371	1.360
8-9	1.433	1.436	1.403	1.438	1.461
9-10	1.418	1.406	1.430	1.407	1.378
10-11	1.350	1.367	1.353	1.390	1.414
11-12	1.473	1.467	1.446	1.443	1.419
12-13	1.352	1.355	1.343	1.367	1.406
13-14	1.476	1.465	1.454	1.445	1.417
13-13^1	----	----	----	----	1.429
13^1-13^2	----	----	----	----	1.569
13^2-15	----	----	----	----	1.534
14-15	1.415	1.403	1.424	1.413	1.396
15-16	1.359	1.372	1.361	1.382	1.364
16-17	1.519	1.506	1.518	1.523	1.523
17-18	1.539	1.533	1.531	1.541	1.555
18-19	1.519	1.506	1.518	1.524	1.525
19-20	1.358	1.372	1.361	1.382	1.382
20-1	1.415	1.403	1.424	1.413	1.388
NA-1	1.349	1.389	1.319	1.362	1.377
NA-4	1.430	1.434	1.392	1.386	1.385
NB-6	1.386	1.383	1.353	1.373	1.361
NB-9	1.386	1.383	1.353	1.373	1.389
NC-11	1.430	1.434	1.393	1.386	1.403
NC-14	1.349	1.389	1.318	1.362	1.347
ND-16	1.388	1.387	1.355	1.364	1.388
ND-19	1.389	1.387	1.356	1.364	1.349
Mg-NA	2.059	1.887	2.055	2.056	2.063
Mg-NB	2.065	1.841	2.063	2.071	2.093
Mg-NC	2.060	1.887	2.055	2.057	2.022
Mg-ND	2.072	2.466	2.100	2.127	2.167
A,B,C,Mg	0.000	0.000	0.000	0.000	0.385
NA-NB	2.922	2.858	2.923	2.922	2.922
NA-NC	4.119	3.716	4.110	4.113	4.011
NA-ND	2.916	2.831	2.927	2.956	2.954
NB-NC	2.922	2.858	2.924	2.922	2.782
NB-ND	4.137	4.307	4.163	4.198	4.191
NC-ND	2.916	2.831	2.926	2.955	2.946

a) 1 is C1; NA is nitrogen in ring A; A,B,C,Mg is the distance between plane NA-NB-NC and the Mg-atom.
b) From ref. 40.
c) From ref. 84.

Table 3S: Calculated heavy atom distances in Mg-BC.

Mg-BC distance[a)]	PM5[b)]	PM3[b)]	HF/6-31G*[c)]	B3LYP/6-31G*[c)]	exp.[d)]
1-2	1.494	1.472	1.383	1.436	1.451
2-3	1.341	1.348	1.399	1.372	1.344
3-4	1.494	1.485	1.383	1.436	1.475
4-5	1.355	1.387	1.449	1.407	1.368
5-6	1.419	1.386	1.333	1.385	1.418
6-7	1.519	1.513	1.520	1.523	1.463
7-8	1.539	1.537	1.535	1.543	1.360
8-9	1.517	1.506	1.514	1.524	1.461
9-10	1.340	1.346	1.428	1.384	1.378
10-11	1.425	1.429	1.358	1.406	1.414
11-12	1.420	1.427	1.474	1.436	1.419
12-13	1.395	1.386	1.327	1.372	1.406
13-14	1.420	1.420	1.473	1.436	1.417
13-13^1	----	----	----	----	1.429
13^1-13^2	----	----	----	----	1.569
13^2-15	----	----	----	----	1.534
14-15	1.426	1.423	1.358	1.407	1.396
15-16	1.339	1.347	1.428	1.384	1.364
16-17	1.517	1.505	1.514	1.524	1.523
17-18	1.540	1.532	1.535	1.543	1.555
18-19	1.518	1.507	1.521	1.524	1.525
19-20	1.419	1.427	1.333	1.384	1.382
20-1	1.355	1.352	1.448	1.407	1.388
NA-1	1.396	1.459	1.361	1.376	1.377
NA-4	1.397	1.377	1.361	1.376	1.385
NB-6	1.330	1.347	1.407	1.361	1.361
NB-9	1.431	1.417	1.292	1.361	1.389
NC-11	1.388	1.398	1.362	1.376	1.403
NC-14	1.388	1.414	1.362	1.376	1.347
ND-16	1.430	1.435	1.292	1.362	1.388
ND-19	1.329	1.332	1.408	1.362	1.349
Mg-NA	2.060	1.881	2.013	2.048	2.063
Mg-NB	2.097	1.837	2.136	2.140	2.093
Mg-NC	2.036	1.885	2.056	2.046	2.022
Mg-ND	2.097	2.505	2.136	2.139	2.167
A,B,C,Mg	0.002	0.005	0.002	0.001	0.385
NA-NB	2.906	2.889	2.974	2.962	2.922
NA-NC	4.096	3.697	4.068	4.094	4.011
NA-ND	2.905	2.801	2.974	2.961	2.954
NB-NC	2.956	2.849	2.924	2.961	2.782
NB-ND	4.193	4.341	4.270	4.279	4.191
NC-ND	2.957	2.865	2.924	2.961	2.946

a) 1 is C1; NA is nitrogen in ring A; A,B,C,Mg is the distance between plane NA-NB-NC and the Mg-atom.
b) From ref. 40.
c) From ref. 41.
d) From ref. 84.

Table 4S: Calculated heavy atom distances in Chl *a*.

Chl *a* distance[a)]	PM5[b)]	PM3[b)]	HF/6-31G*	B3LYP/6-31G*	exp.[c)]
1-2	1.492	1.473	1.482	1.452	1.451
2-3	1.357	1.372	1.339	1.383	1.344
3-4	1.490	1.478	1.480	1.461	1.475
4-5	1.343	1.355	1.351	1.391	1.368
5-6	1.435	1.433	1.446	1.411	1.418
6-7	1.452	1.452	1.447	1.450	1.463
7-8	1.379	1.380	1.359	1.378	1.360
8-9	1.451	1.452	1.448	1.452	1.461
9-10	1.383	1.394	1.368	1.405	1.378
10-11	1.382	1.393	1.416	1.399	1.414
11-12	1.453	1.454	1.406	1.451	1.419
12-13	1.383	1.389	1.403	1.390	1.406
13-14	1.453	1.446	1.389	1.420	1.417
13-13^1	1.438	1.463	1.452	1.461	1.429
13^1-13^2	1.582	1.568	1.564	1.585	1.569
13^2-15	1.520	1.525	1.535	1.536	1.534
14-15	1.435	1.424	1.444	1.414	1.396
15-16	1.345	1.366	1.339	1.381	1.364
16-17	1.520	1.525	1.520	1.523	1.523
17-18	1.560	1.556	1.542	1.550	1.555
18-19	1.529	1.519	1.520	1.526	1.525
19-20	1.383	1.361	1.409	1.391	1.382
20-1	1.392	1.434	1.383	1.410	1.388
NA-1	1.358	1.348	1.338	1.364	1.377
NA-4	1.424	1.442	1.376	1.379	1.385
NB-6	1.360	1.366	1.313	1.365	1.361
NB-9	1.417	1.428	1.391	1.378	1.389
NC-11	1.425	1.434	1.385	1.394	1.403
NC-14	1.330	1.343	1.310	1.335	1.347
ND-16	1.421	1.387	1.403	1.377	1.388
ND-19	1.361	1.410	1.311	1.358	1.349
Mg-NA	2.030	2.370	2.020	2.030	2.063
Mg-NB	2.088	2.438	2.077	2.073	2.093
Mg-NC	2.029	1.835	2.001	2.018	2.022
Mg-ND	2.101	1.821	2.132	2.149	2.167
A,B,C,Mg	0.007	0.123	0.027	0.008	0.385
NA-NB	2.943	3.019	2.917	2.941	2.922
NA-NC	4.058	4.112	4.020	4.048	4.011
NA-ND	2.956	2.897	2.946	2.986	2.954
NB-NC	2.812	2.745	2.837	2.826	2.782
NB-ND	4.189	4.209	4.208	4.221	4.191
NC-ND	2.955	3.101	2.942	2.945	2.946

a) 1 is C1; NA is nitrogen in ring A; A,B,C,Mg is the distance between plane NA-NB-NC and the Mg-atom.
b) From ref. 40.
c) From ref. 84.

Table 5S: Calculated heavy atom distances in Chl *b*.

Chl *b* distance[a)]	PM5[b)]	PM3[b)]	HF/6-31G*	B3LYP/6-31G*	exp.[c)]
1-2	1.492	1.470	1.476	1.454	1.451
2-3	1.356	1.373	1.343	1.381	1.344
3-4	1.489	1.478	1.476	1.463	1.475
4-5	1.341	1.355	1.344	1.385	1.368
5-6	1.438	1.436	1.453	1.418	1.418
6-7	1.449	1.454	1.431	1.450	1.463
7-8	1.400	1.388	1.390	1.394	1.360
8-9	1.430	1.444	1.411	1.439	1.461
9-10	1.400	1.402	1.405	1.409	1.378
10-11	1.367	1.384	1.378	1.394	1.414
11-12	1.467	1.461	1.436	1.454	1.419
12-13	1.374	1.384	1.378	1.388	1.406
13-14	1.464	1.450	1.408	1.421	1.417
13-13^1	1.442	1.465	1.460	1.462	1.429
13^1-13^2	1.582	1.567	1.564	1.584	1.569
13^2-15	1.518	1.524	1.537	1.536	1.534
14-15	1.433	1.422	1.436	1.416	1.396
15-16	1.348	1.368	1.348	1.380	1.364
16-17	1.520	1.525	1.518	1.522	1.523
17-18	1.562	1.556	1.542	1.550	1.555
18-19	1.529	1.519	1.521	1.525	1.525
19-20	1.378	1.359	1.387	1.390	1.382
20-1	1.396	1.436	1.403	1.411	1.388
NA-1	1.355	1.347	1.325	1.362	1.377
NA-4	1.427	1.449	1.388	1.383	1.385
NB-6	1.358	1.365	1.321	1.359	1.361
NB-9	1.418	1.424	1.384	1.385	1.389
NC-11	1.431	1.440	1.394	1.396	1.403
NC-14	1.325	1.341	1.302	1.334	1.347
ND-16	1.416	1.384	1.385	1.379	1.388
ND-19	1.367	1.411	1.331	1.358	1.349
Mg-NA	2.028	2.380	2.014	2.026	2.063
Mg-NB	2.089	2.431	2.082	2.082	2.093
Mg-NC	2.032	1.836	2.010	2.019	2.022
Mg-ND	2.101	1.821	2.124	2.146	2.167
A,B,C,Mg	0.010	0.111	0.019	0.012	0.385
NA-NB	2.948	3.006	2.934	2.944	2.922
NA-NC	4.059	4.119	4.023	4.045	4.011
NA-ND	2.956	2.916	2.944	2.981	2.954
NB-NC	2.816	2.749	2.840	2.834	2.782
NB-ND	4.189	4.201	4.205	4.227	4.191
NC-ND	2.948	3.093	2.923	2.945	2.946

a) 1 is C1; NA is nitrogen in ring A; A,B,C,Mg is the distance between plane NA-NB-NC and the Mg-atom.
b) From ref. 40.
c) From ref. 84.

Table 6S: Calculated heavy atom distances in Chl c_1.

Chl c_1 distance[a)]	PM5[b)]	PM3[b)]	HF/6-31G*	B3LYP/6-31G*	exp.[c)]
1-2	1.495	1.464	1.475	1.451	1.451
2-3	1.354	1.377	1.340	1.380	1.344
3-4	1.493	1.473	1.483	1.464	1.475
4-5	1.347	1.364	1.361	1.400	1.368
5-6	1.432	1.427	1.431	1.403	1.418
6-7	1.467	1.456	1.460	1.458	1.463
7-8	1.369	1.380	1.351	1.372	1.360
8-9	1.467	1.452	1.459	1.459	1.461
9-10	1.364	1.399	1.359	1.399	1.378
10-11	1.404	1.388	1.429	1.405	1.414
11-12	1.442	1.460	1.408	1.456	1.419
12-13	1.392	1.384	1.398	1.385	1.406
13-14	1.444	1.453	1.388	1.422	1.417
13-13^1	1.436	1.464	1.453	1.460	1.429
13^1-13^2	1.588	1.570	1.569	1.590	1.569
13^2-15	1.519	1.520	1.534	1.533	1.534
14-15	1.435	1.425	1.434	1.404	1.396
15-16	1.343	1.373	1.357	1.405	1.364
16-17	1.481	1.491	1.465	1.461	1.523
17-18	1.355	1.371	1.349	1.386	1.555
18-19	1.493	1.481	1.466	1.449	1.525
19-20	1.396	1.365	1.421	1.406	1.382
20-1	1.378	1.432	1.371	1.398	1.388
NA-1	1.373	1.355	1.351	1.372	1.377
NA-4	1.414	1.439	1.364	1.369	1.385
NB-6	1.351	1.373	1.316	1.367	1.361
NB-9	1.428	1.414	1.390	1.376	1.389
NC-11	1.412	1.432	1.369	1.382	1.403
NC-14	1.339	1.345	1.320	1.344	1.347
ND-16	1.437	1.397	1.396	1.380	1.388
ND-19	1.360	1.412	1.319	1.371	1.349
Mg-NA	2.026	2.370	2.018	2.036	2.063
Mg-NB	2.080	2.416	2.071	2.075	2.093
Mg-NC	2.032	1.831	2.007	2.020	2.022
Mg-ND	2.085	1.813	2.100	2.104	2.167
A,B,C,Mg	0.005	0.098	0.002	0.001	0.385
NA-NB	2.941	3.008	2.905	2.929	2.922
NA-NC	4.057	4.124	4.024	4.055	4.011
NA-ND	2.926	2.948	2.946	2.983	2.954
NB-NC	2.816	2.781	2.835	2.826	2.782
NB-ND	4.165	4.194	4.170	4.178	4.191
NC-ND	2.944	3.026	2.906	2.908	2.946

a) 1 is C1; NA is nitrogen in ring A; A,B,C,Mg is the distance between plane NA-NB-NC and the Mg-atom.
b) From ref. 40.
c) From ref. 84.

Table 7S: Calculated heavy atom distances in Chl c_2.

Chl c_2 distance[a)]	PM5[b)]	PM3[b)]	HF/6-31G*	B3LYP/6-31G*	exp.[c)]
1-2	1.494	1.471	1.475	1.452	1.451
2-3	1.356	1.375	1.341	1.380	1.344
3-4	1.492	1.476	1.482	1.464	1.475
4-5	1.346	1.363	1.360	1.399	1.368
5-6	1.432	1.426	1.433	1.405	1.418
6-7	1.461	1.451	1.453	1.451	1.463
7-8	1.375	1.384	1.355	1.379	1.360
8-9	1.461	1.452	1.457	1.464	1.461
9-10	1.370	1.402	1.363	1.401	1.378
10-11	1.398	1.387	1.424	1.404	1.414
11-12	1.445	1.462	1.410	1.456	1.419
12-13	1.389	1.383	1.397	1.385	1.406
13-14	1.448	1.453	1.390	1.423	1.417
13-13^1	1.438	1.464	1.452	1.460	1.429
13^1-13^2	1.587	1.569	1.570	1.591	1.569
13^2-15	1.518	1.521	1.535	1.533	1.534
14-15	1.436	1.425	1.434	1.404	1.396
15-16	1.342	1.374	1.355	1.404	1.364
16-17	1.481	1.494	1.467	1.461	1.523
17-18	1.355	1.373	1.348	1.384	1.555
18-19	1.495	1.481	1.467	1.449	1.525
19-20	1.392	1.366	1.418	1.405	1.382
20-1	1.383	1.432	1.374	1.397	1.388
NA-1	1.369	1.355	1.348	1.372	1.377
NA-4	1.417	1.431	1.366	1.370	1.385
NB-6	1.355	1.376	1.318	1.369	1.361
NB-9	1.422	1.415	1.387	1.375	1.389
NC-11	1.415	1.432	1.372	1.383	1.403
NC-14	1.336	1.344	1.318	1.343	1.347
ND-16	1.435	1.396	1.396	1.381	1.388
ND-19	1.363	1.412	1.320	1.371	1.349
Mg-NA	2.027	2.360	2.018	2.035	2.063
Mg-NB	2.079	2.423	2.075	2.079	2.093
Mg-NC	2.033	1.829	2.007	2.018	2.022
Mg-ND	2.083	1.814	2.099	2.106	2.167
A,B,C,Mg	0.016	0.093	0.014	0.007	0.385
NA-NB	2.943	3.030	2.909	2.935	2.922
NA-NC	4.059	4.115	4.025	4.053	4.011
NA-ND	2.926	2.929	2.946	2.982	2.954
NB-NC	2.816	2.777	2.836	2.827	2.782
NB-ND	4.162	4.205	4.172	4.183	4.191
NC-ND	2.941	3.029	2.904	2.907	2.946

a) 1 is C1; NA is nitrogen in ring A; A,B,C,Mg is the distance between plane NA-NB-NC and the Mg-atom.
b) From ref. 40.
c) From ref. 84.

Table 8S: Calculated heavy atom distances in Chl c_3.

Chl c_3 distance[a)]	PM5[b)]	PM3[b)]	HF/6-31G*	B3LYP/6-31G*	exp.[c)]
1-2	1.488	1.472	1.471	1.453	1.451
2-3	1.359	1.375	1.344	1.379	1.344
3-4	1.489	1.477	1.478	1.468	1.475
4-5	1.342	1.359	1.351	1.395	1.368
5-6	1.438	1.433	1.446	1.411	1.418
6-7	1.446	1.449	1.438	1.453	1.463
7-8	1.400	1.394	1.383	1.392	1.360
8-9	1.430	1.443	1.425	1.455	1.461
9-10	1.406	1.408	1.393	1.404	1.378
10-11	1.363	1.382	1.390	1.398	1.414
11-12	1.474	1.466	1.428	1.457	1.419
12-13	1.371	1.381	1.383	1.384	1.406
13-14	1.464	1.456	1.402	1.424	1.417
13-13^1	1.444	1.464	1.456	1.460	1.429
13^1-13^2	1.581	1.569	1.570	1.590	1.569
13^2-15	1.516	1.521	1.536	1.533	1.534
14-15	1.431	1.426	1.437	1.407	1.396
15-16	1.349	1.375	1.354	1.401	1.364
16-17	1.487	1.495	1.477	1.464	1.523
17-18	1.352	1.372	1.343	1.383	1.555
18-19	1.499	1.482	1.477	1.452	1.525
19-20	1.369	1.364	1.394	1.404	1.382
20-1	1.406	1.434	1.396	1.399	1.388
NA-1	1.352	1.352	1.331	1.369	1.377
NA-4	1.428	1.435	1.380	1.372	1.385
NB-6	1.363	1.370	1.322	1.364	1.361
NB-9	1.411	1.418	1.380	1.377	1.389
NC-11	1.431	1.436	1.383	1.385	1.403
NC-14	1.326	1.342	1.308	1.342	1.347
ND-16	1.419	1.395	1.390	1.381	1.388
ND-19	1.384	1.415	1.333	1.370	1.349
Mg-NA	2.029	2.361	2.015	2.030	2.063
Mg-NB	2.082	2.424	2.085	2.089	2.093
Mg-NC	2.037	1.829	2.009	2.019	2.022
Mg-ND	2.079	1.814	2.089	2.106	2.167
A,B,C,Mg	0.014	0.095	0.012	0.013	0.385
NA-NB	2.956	3.036	2.925	2.938	2.922
NA-NC	4.065	4.117	4.024	4.048	4.011
NA-ND	2.929	2.925	2.937	2.977	2.954
NB-NC	2.826	2.776	2.848	2.839	2.782
NB-ND	4.159	4.206	4.173	4.193	4.191
NC-ND	2.920	3.029	2.886	2.905	2.946

a) 1 is C1; NA is nitrogen in ring A; A,B,C,Mg is the distance between plane NA-NB-NC and the Mg-atom.
b) From ref. 40.
c) From ref. 84.

Table 9S: Calculated heavy atom distances in Chl *d*.

Chl *d* distance[a)]	PM5[b)]	PM3[b)]	HF/6-31G*	B3LYP/6-31G*	exp.[c)]
1-2	1.497	1.474	1.484	1.446	1.451
2-3	1.363	1.371	1.343	1.387	1.344
3-4	1.487	1.471	1.477	1.457	1.475
4-5	1.343	1.359	1.352	1.397	1.368
5-6	1.434	1.428	1.445	1.408	1.418
6-7	1.455	1.451	1.445	1.451	1.463
7-8	1.377	1.381	1.360	1.377	1.360
8-9	1.455	1.450	1.446	1.453	1.461
9-10	1.378	1.400	1.370	1.407	1.378
10-11	1.387	1.387	1.414	1.397	1.414
11-12	1.449	1.459	1.408	1.455	1.419
12-13	1.385	1.385	1.402	1.388	1.406
13-14	1.451	1.449	1.389	1.422	1.417
13-13^1	1.437	1.464	1.453	1.463	1.429
13^1-13^2	1.583	1.568	1.565	1.583	1.569
13^2-15	1.520	1.526	1.535	1.536	1.534
14-15	1.436	1.421	1.443	1.411	1.396
15-16	1.343	1.368	1.338	1.384	1.364
16-17	1.518	1.526	1.519	1.523	1.523
17-18	1.560	1.556	1.543	1.551	1.555
18-19	1.529	1.518	1.520	1.526	1.525
19-20	1.390	1.360	1.411	1.387	1.382
20-1	1.384	1.434	1.379	1.412	1.388
NA-1	1.363	1.350	1.339	1.367	1.377
NA-4	1.422	1.439	1.377	1.376	1.385
NB-6	1.357	1.372	1.315	1.367	1.361
NB-9	1.419	1.420	1.389	1.375	1.389
NC-11	1.423	1.436	1.385	1.393	1.403
NC-14	1.331	1.342	1.311	1.337	1.347
ND-16	1.425	1.385	1.404	1.374	1.388
ND-19	1.353	1.411	1.308	1.361	1.349
Mg-NA	2.033	2.372	2.025	2.034	2.063
Mg-NB	2.086	2.435	2.072	2.072	2.093
Mg-NC	2.031	1.834	2.000	2.018	2.022
Mg-ND	2.104	1.821	2.137	2.151	2.167
A,B,C,Mg	0.012	0.118	0.032	0.009	0.385
NA-NB	2.942	3.019	2.917	2.941	2.922
NA-NC	4.062	4.114	4.025	4.052	4.011
NA-ND	2.962	2.902	2.956	2.995	2.954
NB-NC	2.812	2.744	2.835	2.825	2.782
NB-ND	4.189	4.207	4.209	4.222	4.191
NC-ND	2.956	3.097	2.941	2.946	2.946

a) 1 is C1; NA is nitrogen in ring A; A,B,C,Mg is the distance between plane NA-NB-NC and the Mg-atom.
b) From ref. 40.
c) From ref. 84.

Table 10S: Calculated heavy atom distances in Bchl *a*.

Bchl *a* distance[a]	PM5[b]	PM3[b]	HF/6-31G*[c]	B3LYP/6-31G*[c]	exp.[d]
1-2	1.412	1.423	1.487	1.443	1.451
2-3	1.418	1.407	1.338	1.396	1.344
3-4	1.427	1.438	1.487	1.456	1.475
4-5	1.434	1.432	1.355	1.408	1.368
5-6	1.339	1.354	1.438	1.390	1.418
6-7	1.528	1.517	1.517	1.524	1.463
7-8	1.557	1.548	1.541	1.550	1.360
8-9	1.527	1.517	1.522	1.527	1.461
9-10	1.436	1.446	1.335	1.388	1.378
10-11	1.346	1.355	1.454	1.410	1.414
11-12	1.518	1.495	1.385	1.447	1.419
12-13	1.346	1.363	1.423	1.392	1.406
13-14	1.491	1.475	1.373	1.417	1.417
13-13^1	1.459	1.473	1.447	1.461	1.429
13^1-13^2	1.576	1.564	1.565	1.584	1.569
13^2-15	1.515	1.523	1.532	1.534	1.534
14-15	1.371	1.388	1.447	1.407	1.396
15-16	1.411	1.402	1.334	1.386	1.364
16-17	1.521	1.527	1.518	1.523	1.523
17-18	1.560	1.557	1.543	1.550	1.555
18-19	1.526	1.516	1.519	1.527	1.525
19-20	1.338	1.356	1.430	1.388	1.382
20-1	1.432	1.430	1.363	1.410	1.388
NA-1	1.394	1.400	1.352	1.374	1.377
NA-4	1.376	1.380	1.367	1.370	1.385
NB-6	1.432	1.438	1.290	1.357	1.361
NB-9	1.326	1.336	1.418	1.369	1.389
NC-11	1.412	1.445	1.381	1.386	1.403
NC-14	1.358	1.353	1.324	1.345	1.347
ND-16	1.340	1.346	1.416	1.371	1.388
ND-19	1.429	1.431	1.294	1.359	1.349
Mg-NA	2.020	2.325	2.031	2.036	2.063
Mg-NB	2.123	2.467	2.115	2.121	2.093
Mg-NC	2.040	1.830	1.988	2.017	2.022
Mg-ND	2.113	1.829	2.149	2.154	2.167
A,B,C,Mg	0.029	0.096	0.087	0.024	0.385
NA-NB	2.992	3.052	2.935	2.984	2.922
NA-NC	4.058	4.067	4.015	4.053	4.011
NA-ND	3.021	2.928	2.954	3.002	2.954
NB-NC	2.786	2.732	2.868	2.846	2.782
NB-ND	4.229	4.268	4.263	4.273	4.191
NC-ND	2.928	3.074	2.963	2.950	2.946

a) 1 is C1; NA is nitrogen in ring A; A,B,C,Mg is the distance between plane NA-NB-NC and the Mg-atom.
b) From ref. 40.
c) From ref. 41.
d) From ref. 84.

Table 11S: Calculated heavy atom distances in Bchl *b*.

Bchl *b* distance[a]	PM5[b]	PM3[b]	HF/6-31G*[c]	B3LYP/6-31G*[c]	exp.[d]
1-2	1.503	1.484	1.487	1.444	1.451
2-3	1.350	1.364	1.335	1.396	1.344
3-4	1.493	1.478	1.483	1.458	1.475
4-5	1.350	1.353	1.355	1.404	1.368
5-6	1.429	1.443	1.438	1.393	1.418
6-7	1.532	1.526	1.514	1.521	1.463
7-8	1.518	1.509	1.518	1.524	1.360
8-9	1.483	1.471	1.483	1.476	1.461
9-10	1.346	1.363	1.342	1.396	1.378
10-11	1.425	1.424	1.448	1.406	1.414
11-12	1.422	1.430	1.388	1.448	1.419
12-13	1.406	1.407	1.420	1.392	1.406
13-14	1.433	1.428	1.375	1.418	1.417
13-13^1	1.430	1.459	1.448	1.460	1.429
13^1-13^2	1.589	1.572	1.565	1.583	1.569
13^2-15	1.522	1.525	1.532	1.535	1.534
14-15	1.438	1.430	1.447	1.408	1.396
15-16	1.337	1.357	1.333	1.384	1.364
16-17	1.518	1.523	1.518	1.523	1.523
17-18	1.561	1.556	1.542	1.551	1.555
18-19	1.529	1.521	1.518	1.527	1.525
19-20	1.416	1.374	1.430	1.388	1.382
20-1	1.360	1.420	1.363	1.409	1.388
NA-1	1.384	1.354	1.354	1.373	1.377
NA-4	1.403	1.445	1.365	1.371	1.385
NB-6	1.326	1.330	1.289	1.352	1.361
NB-9	1.442	1.453	1.423	1.383	1.389
NC-11	1.407	1.418	1.381	1.387	1.403
NC-14	1.346	1.356	1.323	1.343	1.347
ND-16	1.441	1.403	1.416	1.372	1.388
ND-19	1.334	1.388	1.294	1.358	1.349
Mg-NA	2.032	2.372	2.025	2.035	2.063
Mg-NB	2.110	2.454	2.123	2.127	2.093
Mg-NC	2.015	1.832	1.985	2.014	2.022
Mg-ND	2.121	1.821	2.154	2.160	2.167
A,B,C,Mg	0.013	0.134	0.081	0.012	0.385
NA-NB	2.947	3.026	2.946	2.998	2.922
NA-NC	4.046	4.116	4.007	4.049	4.011
NA-ND	2.951	2.893	2.947	2.997	2.954
NB-NC	2.833	2.769	2.872	2.851	2.782
NB-ND	4.231	4.226	4.277	4.285	4.191
NC-ND	2.978	3.106	2.961	2.945	2.946

a) 1 is C1; NA is nitrogen in ring A; A,B,C,Mg is the distance between plane NA-NB-NC and the Mg-atom.
b) From ref. 40.
c) From ref. 41.
d) From ref. 84.

Table 12S: Calculated heavy atom distances in Bchl *c*.

Bchl *c* distance[a)]	PM5[b)]	PM3[b)]	HF/6-31G*	B3LYP/6-31G*	exp.[c)]
1-2	1.497	1.477	1.501	1.468	1.451
2-3	1.358	1.372	1.340	1.379	1.344
3-4	1.480	1.467	1.470	1.447	1.475
4-5	1.342	1.360	1.354	1.397	1.368
5-6	1.431	1.426	1.441	1.405	1.418
6-7	1.445	1.452	1.443	1.449	1.463
7-8	1.386	1.381	1.362	1.379	1.360
8-9	1.444	1.448	1.443	1.452	1.461
9-10	1.397	1.400	1.373	1.405	1.378
10-11	1.368	1.384	1.407	1.397	1.414
11-12	1.466	1.463	1.413	1.455	1.419
12-13	1.376	1.385	1.396	1.388	1.406
13-14	1.459	1.450	1.393	1.422	1.417
13-13^1	1.445	1.468	1.461	1.468	1.429
13^1-13^2	1.562	1.552	1.554	1.570	1.569
13^2-15	1.514	1.519	1.527	1.527	1.534
14-15	1.430	1.417	1.439	1.409	1.396
15-16	1.343	1.365	1.337	1.381	1.364
16-17	1.517	1.520	1.510	1.515	1.523
17-18	1.556	1.553	1.536	1.545	1.555
18-19	1.536	1.525	1.533	1.538	1.525
19-20	1.389	1.371	1.421	1.403	1.382
20-1	1.412	1.455	1.403	1.434	1.388
NA-1	1.357	1.353	1.345	1.369	1.377
NA-4	1.431	1.450	1.379	1.383	1.385
NB-6	1.365	1.369	1.314	1.365	1.361
NB-9	1.409	1.417	1.386	1.377	1.389
NC-11	1.429	1.440	1.385	1.392	1.403
NC-14	1.324	1.339	1.308	1.336	1.347
ND-16	1.416	1.386	1.404	1.377	1.388
ND-19	1.368	1.413	1.318	1.366	1.349
Mg-NA	2.038	2.393	2.030	2.039	2.063
Mg-NB	2.078	2.424	2.072	2.070	2.093
Mg-NC	2.043	1.841	2.011	2.025	2.022
Mg-ND	2.095	1.819	2.109	2.130	2.167
A,B,C,Mg	0.053	0.059	0.006	0.017	0.385
NA-NB	2.996	3.078	2.972	2.991	2.922
NA-NC	4.079	4.148	4.041	4.064	4.011
NA-ND	2.915	2.869	2.896	2.936	2.954
NB-NC	2.769	2.703	2.804	2.799	2.782
NB-ND	4.171	4.202	4.180	4.199	4.191
NC-ND	2.986	3.144	2.955	2.961	2.946

a) 1 is C1; NA is nitrogen in ring A; A,B,C,Mg is the distance between plane NA-NB-NC and the Mg-atom.
b) From ref. 40.
c) From ref. 84.

Table 13S: Calculated heavy atom distances in **B**chl *d*.

Bchl *d* distance[a)]	PM5[b)]	PM3[b)]	HF/6-31G*	B3LYP/6-31G*	exp.[c)]
1-2	1.497	1.468	1.482	1.456	1.451
2-3	1.353	1.370	1.340	1.376	1.344
3-4	1.492	1.474	1.481	1.458	1.475
4-5	1.344	1.359	1.352	1.392	1.368
5-6	1.435	1.432	1.446	1.412	1.418
6-7	1.458	1.454	1.446	1.450	1.463
7-8	1.374	1.380	1.360	1.378	1.360
8-9	1.459	1.450	1.445	1.452	1.461
9-10	1.377	1.396	1.372	1.405	1.378
10-11	1.389	1.389	1.412	1.398	1.414
11-12	1.449	1.460	1.410	1.452	1.419
12-13	1.386	1.388	1.400	1.390	1.406
13-14	1.450	1.447	1.391	1.421	1.417
13-13^1	1.445	1.469	1.459	1.468	1.429
13^1-13^2	1.562	1.552	1.554	1.569	1.569
13^2-15	1.515	1.517	1.527	1.527	1.534
14-15	1.438	1.422	1.444	1.415	1.396
15-16	1.339	1.364	1.336	1.380	1.364
16-17	1.518	1.524	1.519	1.523	1.523
17-18	1.561	1.558	1.544	1.551	1.555
18-19	1.530	1.519	1.521	1.528	1.525
19-20	1.393	1.361	1.410	1.390	1.382
20-1	1.382	1.434	1.382	1.410	1.388
NA-1	1.364	1.348	1.339	1.361	1.377
NA-4	1.422	1.451	1.378	1.383	1.385
NB-6	1.354	1.368	1.314	1.365	1.361
NB-9	1.421	1.421	1.388	1.378	1.389
NC-11	1.421	1.436	1.385	1.393	1.403
NC-14	1.332	1.341	1.311	1.337	1.347
ND-16	1.428	1.388	1.404	1.378	1.388
ND-19	1.350	1.405	1.308	1.357	1.349
Mg-NA	2.031	2.377	2.020	2.030	2.063
Mg-NB	2.085	2.426	2.075	2.071	2.093
Mg-NC	2.032	1.837	2.001	2.016	2.022
Mg-ND	2.102	1.817	2.132	2.150	2.167
A,B,C,Mg	0.029	0.088	0.032	0.012	0.385
NA-NB	2.939	3.005	2.917	2.938	2.922
NA-NC	4.061	4.123	4.020	4.046	4.011
NA-ND	2.959	2.916	2.951	2.987	2.954
NB-NC	2.800	2.739	2.834	2.826	2.782
NB-ND	4.185	4.202	4.207	4.220	4.191
NC-ND	2.967	3.108	2.938	2.943	2.946

a) 1 is C1; NA is nitrogen in ring A; A,B,C,Mg is the distance between plane NA-NB-NC and the Mg-atom.
b) From ref. 40.
c) From ref. 84.

Table 14S: Calculated heavy atom distances in **B**chl *e*.

Bchl *e* distance[a)]	**PM5**[b)]	**PM3**[b)]	**HF/6-31G***	**B3LYP/6-31G***	**exp.**[c)]
1-2	1.501	1.478	1.498	1.472	1.451
2-3	1.355	1.371	1.341	1.376	1.344
3-4	1.485	1.469	1.469	1.451	1.475
4-5	1.342	1.358	1.349	1.390	1.368
5-6	1.436	1.431	1.450	1.414	1.418
6-7	1.451	1.453	1.427	1.450	1.463
7-8	1.399	1.389	1.393	1.394	1.360
8-9	1.433	1.441	1.410	1.438	1.461
9-10	1.398	1.406	1.406	1.408	1.378
10-11	1.368	1.379	1.376	1.392	1.414
11-12	1.467	1.467	1.439	1.456	1.419
12-13	1.374	1.382	1.381	1.392	1.406
13-14	1.461	1.452	1.408	1.423	1.417
13-13^1	1.452	1.469	1.466	1.412	1.429
13^1-13^2	1.558	1.552	1.553	1.469	1.569
13^2-15	1.515	1.519	1.528	1.567	1.534
14-15	1.432	1.417	1.434	1.526	1.396
15-16	1.342	1.366	1.343	1.378	1.364
16-17	1.514	1.520	1.511	1.514	1.523
17-18	1.559	1.553	1.536	1.544	1.555
18-19	1.536	1.525	1.533	1.538	1.525
19-20	1.398	1.371	1.401	1.404	1.382
20-1	1.403	1.455	1.421	1.432	1.388
NA-1	1.363	1.352	1.332	1.367	1.377
NA-4	1.427	1.451	1.387	1.384	1.385
NB-6	1.356	1.366	1.319	1.357	1.361
NB-9	1.419	1.419	1.384	1.385	1.389
NC-11	1.431	1.443	1.394	1.395	1.403
NC-14	1.325	1.337	1.300	1.334	1.347
ND-16	1.423	1.385	1.390	1.379	1.388
ND-19	1.359	1.414	1.335	1.364	1.349
Mg-NA	2.035	2.391	2.030	2.038	2.063
Mg-NB	2.086	2.427	2.073	2.077	2.093
Mg-NC	2.043	1.840	2.017	2.027	2.022
Mg-ND	2.099	1.820	2.100	2.127	2.167
A,B,C,Mg	0.076	0.048	0.005	0.016	0.385
NA-NB	2.992	3.081	2.981	2.992	2.922
NA-NC	4.074	4.148	4.047	4.065	4.011
NA-ND	2.919	2.866	2.891	2.928	2.954
NB-NC	2.781	2.708	2.812	2.810	2.782
NB-ND	4.182	4.205	4.173	4.203	4.191
NC-ND	2.983	3.143	2.941	2.964	2.946

a) 1 is C1; NA is nitrogen in ring A; A,B,C,Mg is the distance between plane NA-NB-NC and the Mg-atom.
b) From ref. 40.
c) From ref. 84.

Table 15S: Calculated heavy atom distances in **B**chl *f*.

Bchl *f* distance[a)]	**PM5**[b)]	**PM3**[b)]	**HF/6-31G***	**B3LYP/6-31G***	**exp.**[c)]
1-2	1.496	1.469	1.482	1.459	1.451
2-3	1.353	1.370	1.340	1.374	1.344
3-4	1.492	1.476	1.480	1.462	1.475
4-5	1.342	1.357	1.347	1.387	1.368
5-6	1.439	1.435	1.453	1.419	1.418
6-7	1.451	1.453	1.433	1.450	1.463
7-8	1.400	1.388	1.389	1.395	1.360
8-9	1.432	1.443	1.414	1.437	1.461
9-10	1.400	1.404	1.398	1.409	1.378
10-11	1.368	1.383	1.386	1.394	1.414
11-12	1.467	1.465	1.431	1.456	1.419
12-13	1.373	1.384	1.386	1.393	1.406
13-14	1.458	1.451	1.402	1.423	1.417
13-13^1	1.451	1.471	1.464	1.468	1.429
13^1-13^2	1.557	1.552	1.552	1.566	1.569
13^2-15	1.513	1.517	1.528	1.526	1.534
14-15	1.434	1.422	1.441	1.418	1.396
15-16	1.342	1.365	1.340	1.377	1.364
16-17	1.519	1.524	1.519	1.523	1.523
17-18	1.560	1.558	1.542	1.551	1.555
18-19	1.530	1.518	1.521	1.527	1.525
19-20	1.386	1.360	1.398	1.392	1.382
20-1	1.389	1.435	1.392	1.408	1.388
NA-1	1.360	1.347	1.330	1.360	1.377
NA-4	1.426	1.452	1.384	1.384	1.385
NB-6	1.357	1.367	1.319	1.357	1.361
NB-9	1.419	1.421	1.388	1.386	1.389
NC-11	1.430	1.440	1.392	1.394	1.403
NC-14	1.325	1.339	1.304	1.335	1.347
ND-16	1.422	1.387	1.396	1.381	1.388
ND-19	1.357	1.407	1.319	1.354	1.349
Mg-NA	2.030	2.375	2.018	2.028	2.063
Mg-NB	2.083	2.428	2.075	2.079	2.093
Mg-NC	2.037	1.836	2.008	2.018	2.022
Mg-ND	2.103	1.817	2.127	2.147	2.167
A,B,C,Mg	0.035	0.077	0.031	0.014	0.385
NA-NB	2.948	3.006	2.925	2.938	2.922
NA-NC	4.064	4.122	4.025	4.046	4.011
NA-ND	2.955	2.918	2.944	2.978	2.954
NB-NC	2.807	2.745	2.841	2.839	2.782
NB-ND	4.184	4.205	4.202	4.225	4.191
NC-ND	2.958	3.103	2.929	2.947	2.946

a) 1 is C1; NA is nitrogen in ring A; A,B,C,Mg is the distance between plane NA-NB-NC and the Mg-atom.
b) From ref. 40.
c) From ref. 84.

Table 16S: Calculated heavy atom distances in **B**chl *g*.

Bchl *f* distance[a]	**PM5**[b]	**PM3**[b]	**HF/6-31G***[c]	**B3LYP/6-31G***[c]	**exp.**[d]
1-2	1.498	1.477	1.484	1.448	1.451
2-3	1.352	1.370	1.336	1.383	1.344
3-4	1.496	1.483	1.485	1.460	1.475
4-5	1.349	1.351	1.356	1.399	1.368
5-6	1.428	1.444	1.437	1.398	1.418
6-7	1.529	1.523	1.515	1.521	1.463
7-8	1.525	1.515	1.518	1.524	1.360
8-9	1.478	1.469	1.482	1.477	1.461
9-10	1.345	1.362	1.342	1.391	1.378
10-11	1.427	1.425	1.449	1.410	1.414
11-12	1.420	1.429	1.387	1.443	1.419
12-13	1.408	1.408	1.420	1.396	1.406
13-14	1.433	1.430	1.375	1.414	1.417
13-13^1	1.426	1.453	1.448	1.458	1.429
13^1-13^2	1.591	1.576	1.565	1.584	1.569
13^2-15	1.524	1.522	1.532	1.535	1.534
14-15	1.438	1.432	1.448	1.411	1.396
15-16	1.336	1.357	1.333	1.381	1.364
16-17	1.517	1.521	1.519	1.523	1.523
17-18	1.560	1.556	1.543	1.551	1.555
18-19	1.530	1.521	1.520	1.526	1.525
19-20	1.415	1.374	1.429	1.395	1.382
20-1	1.361	1.420	1.363	1.403	1.388
NA-1	1.386	1.355	1.357	1.374	1.377
NA-4	1.403	1.448	1.363	1.371	1.385
NB-6	1.326	1.328	1.290	1.347	1.361
NB-9	1.446	1.460	1.423	1.388	1.389
NC-11	1.407	1.415	1.382	1.389	1.403
NC-14	1.344	1.354	1.323	1.343	1.347
ND-16	1.440	1.405	1.415	1.378	1.388
ND-19	1.334	1.387	1.295	1.352	1.349
Mg-NA	2.030	2.366	2.022	2.026	2.063
Mg-NB	2.116	2.459	2.123	2.134	2.093
Mg-NC	2.017	1.830	1.987	2.008	2.022
Mg-ND	2.123	1.820	2.152	2.162	2.167
A,B,C,Mg	0.019	0.107	0.071	0.015	0.385
NA-NB	2.963	3.040	2.944	2.987	2.922
NA-NC	4.045	4.114	4.006	4.033	4.011
NA-ND	2.947	2.914	2.945	2.985	2.954
NB-NC	2.826	2.774	2.872	2.861	2.782
NB-ND	4.238	4.240	4.274	4.295	4.191
NC-ND	2.982	3.084	2.960	2.953	2.946

a) 1 is C1; NA is nitrogen in ring A; A,B,C,Mg is the distance between plane NA-NB-NC and the Mg-atom.
b) From ref. 40.
c) From ref. 41.
d) From ref. 84.

Table 17S: Calculated heavy atom distances in **B**chl *h*.

Bchl *h* distance[a)]	PM5[b)]	PM3[b)]	HF/6-31G*[c)]	B3LYP/6-31G*[c)]	exp.[d)]
1-2	1.422	1.428	1.484	1.447	1.451
2-3	1.405	1.402	1.337	1.385	1.344
3-4	1.423	1.439	1.485	1.458	1.475
4-5	1.424	1.420	1.358	1.403	1.368
5-6	1.343	1.361	1.435	1.396	1.418
6-7	1.526	1.518	1.517	1.525	1.463
7-8	1.558	1.548	1.542	1.551	1.360
8-9	1.527	1.517	1.522	1.527	1.461
9-10	1.436	1.441	1.335	1.384	1.378
10-11	1.346	1.357	1.455	1.415	1.414
11-12	1.515	1.492	1.385	1.441	1.419
12-13	1.348	1.364	1.424	1.396	1.406
13-14	1.490	1.474	1.374	1.414	1.417
13-13^1	1.459	1.473	1.447	1.459	1.429
13^1-13^2	1.576	1.564	1.565	1.585	1.569
13^2-15	1.515	1.522	1.532	1.535	1.534
14-15	1.373	1.390	1.448	1.412	1.396
15-16	1.408	1.399	1.333	1.381	1.364
16-17	1.521	1.526	1.519	1.523	1.523
17-18	1.561	1.557	1.543	1.551	1.555
18-19	1.526	1.516	1.520	1.527	1.525
19-20	1.340	1.356	1.431	1.395	1.382
20-1	1.430	1.430	1.362	1.403	1.388
NA-1	1.384	1.390	1.358	1.375	1.377
NA-4	1.387	1.394	1.362	1.370	1.385
NB-6	1.428	1.428	1.291	1.352	1.361
NB-9	1.326	1.340	1.417	1.377	1.389
NC-11	1.413	1.445	1.382	1.387	1.403
NC-14	1.355	1.352	1.325	1.345	1.347
ND-16	1.341	1.348	1.417	1.377	1.388
ND-19	1.428	1.427	1.293	1.353	1.349
Mg-NA	2.013	2.331	2.025	2.027	2.063
Mg-NB	2.127	2.463	2.118	2.128	2.093
Mg-NC	2.038	1.830	1.987	2.012	2.022
Mg-ND	2.115	1.827	2.148	2.157	2.167
A,B,C,Mg	0.021	0.076	0.089	0.028	0.385
NA-NB	2.993	3.047	2.933	2.973	2.922
NA-NC	4.049	4.073	4.008	4.038	4.011
NA-ND	3.007	2.947	2.946	2.991	2.954
NB-NC	2.791	2.735	2.870	2.856	2.782
NB-ND	4.236	4.266	4.265	4.283	4.191
NC-ND	2.932	3.063	2.964	2.957	2.946

a) 1 is C1; NA is nitrogen in ring A; A,B,C,Mg is the distance between plane NA-NB-NC and the Mg-atom.
b) From ref. 40.
c) From ref. 41.
d) From ref. 84.