

Supporting Information

for

Designing Biphenanthridine-Based Singlet Fission Materials Using Computational Chemistry

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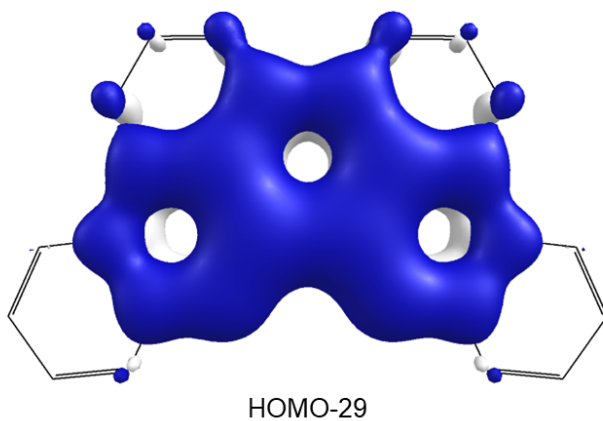


Figure S1. HOMO-29 of **5** illustrating π conjugation across the two phenanthridinyl sub-units.

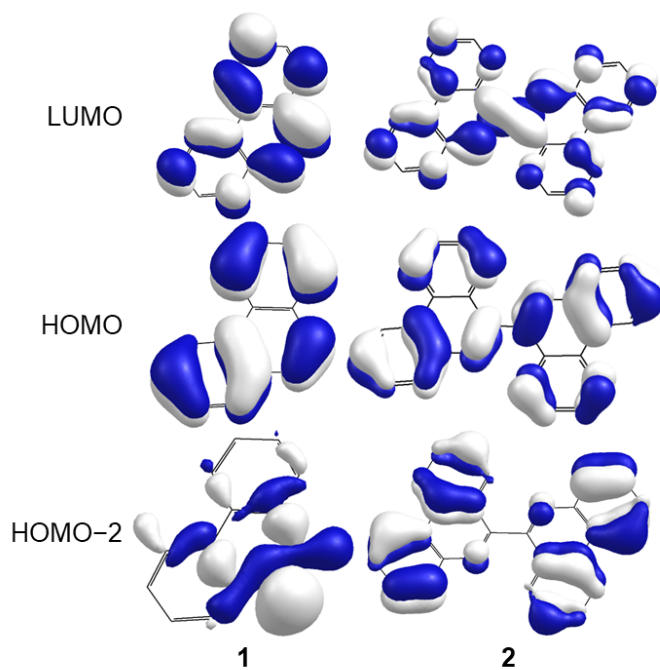


Figure S2. Selected molecular orbitals of **1** and **2**.

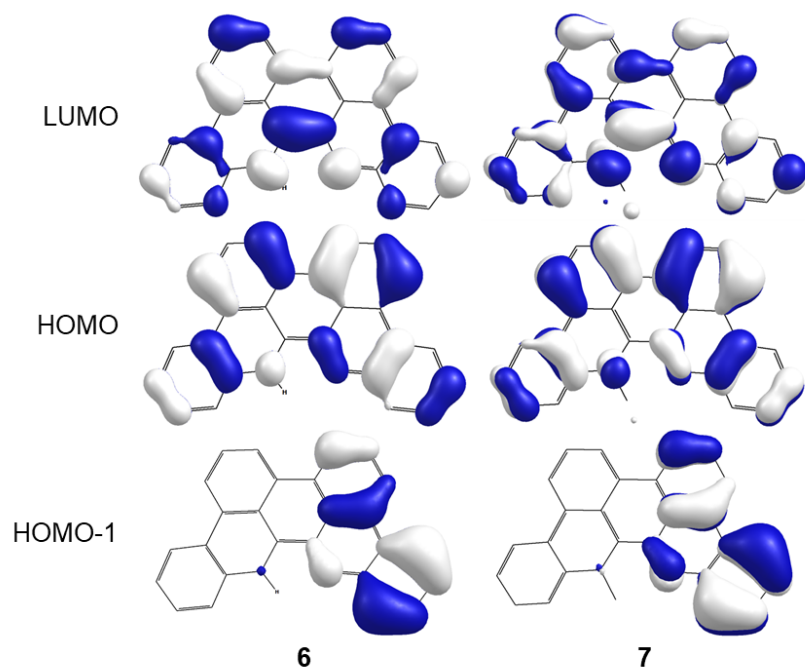


Figure S3. Selected molecular orbitals of **6** and **7**.

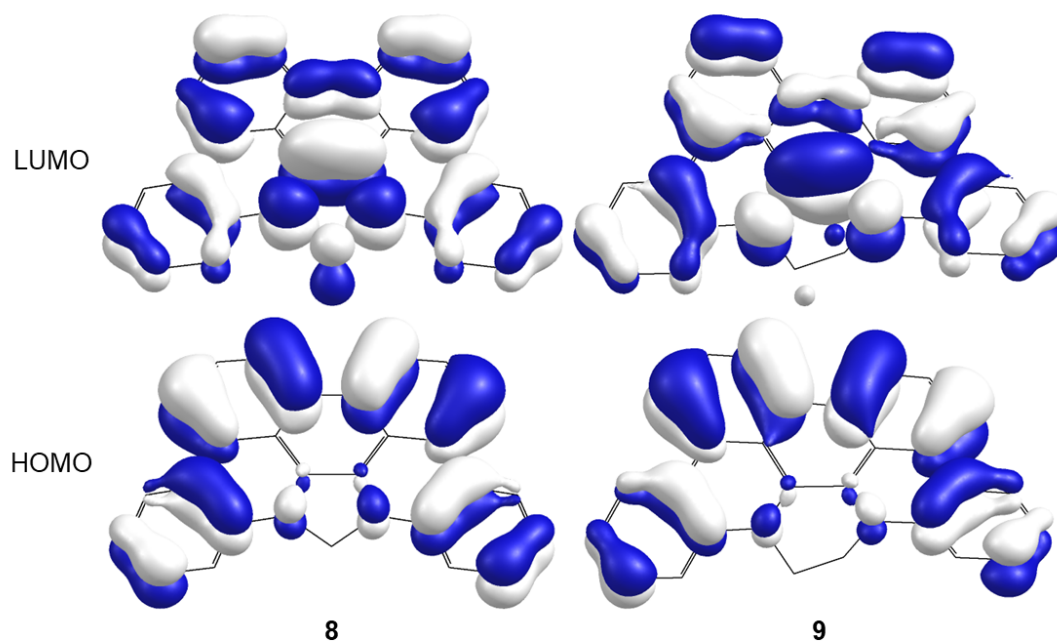


Figure S4. Frontier molecular orbitals of **8** and **9**.

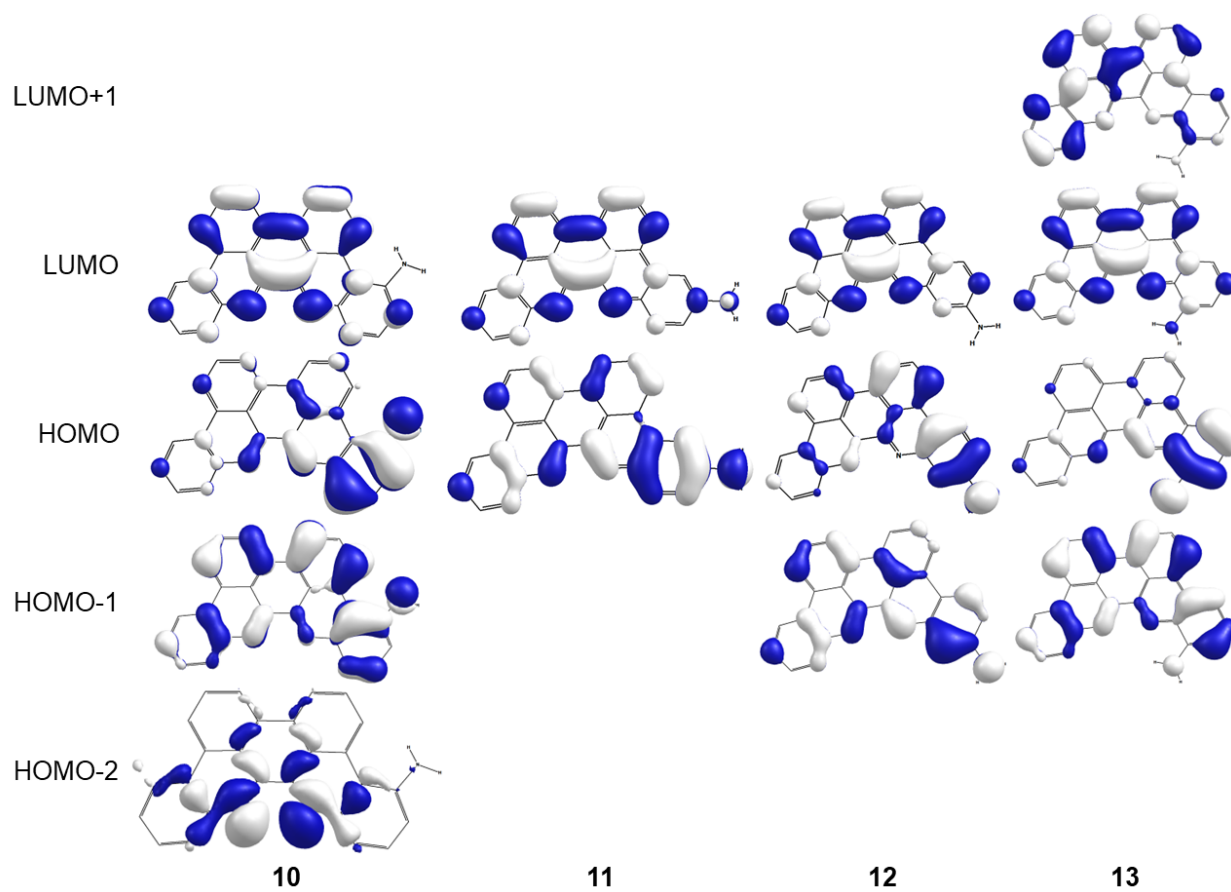


Figure S5. Selected molecular orbitals of **10-13**.

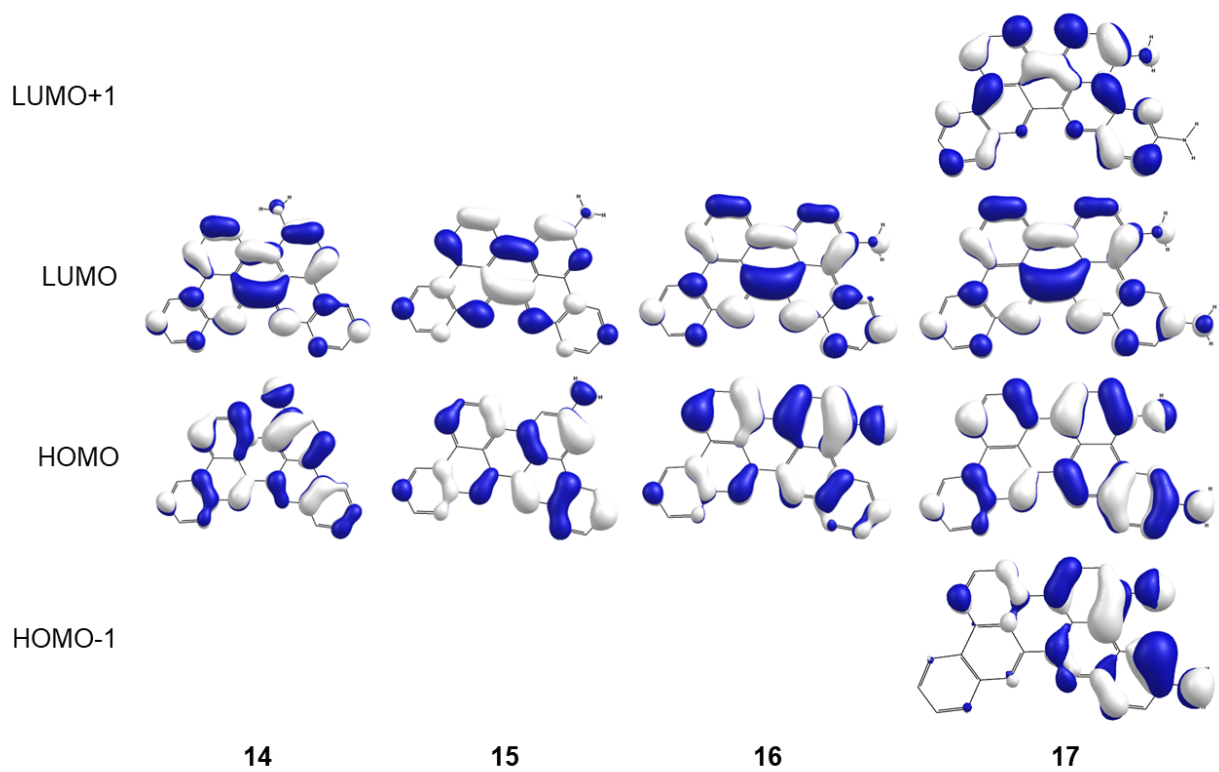


Figure S6. Selected molecular orbitals of 14-17.

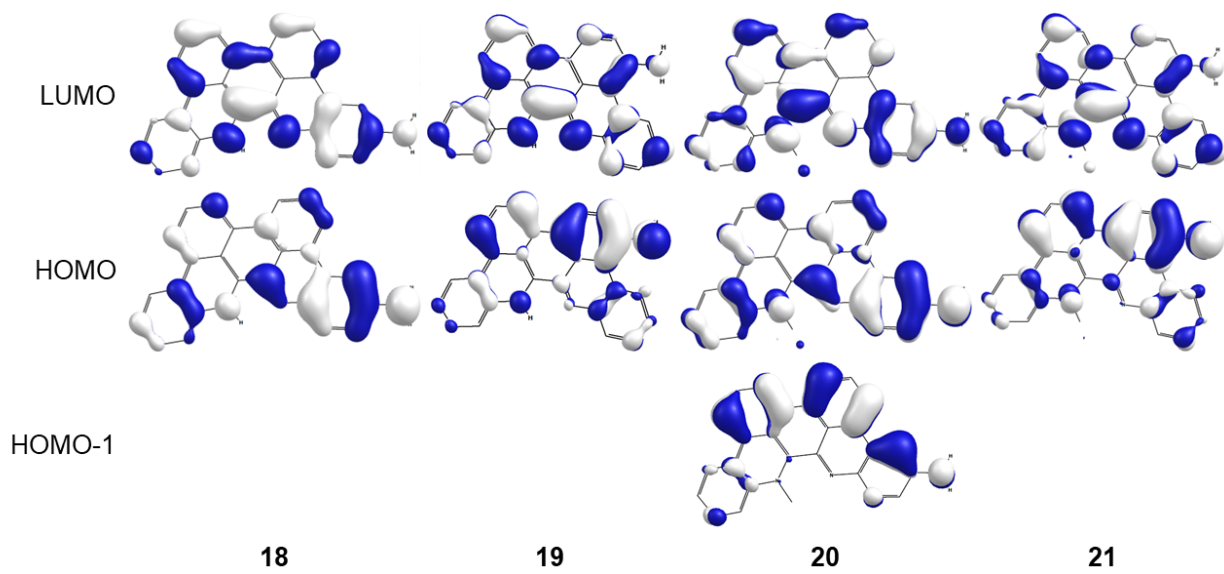


Figure S7. Selected molecular orbitals of 18-21.

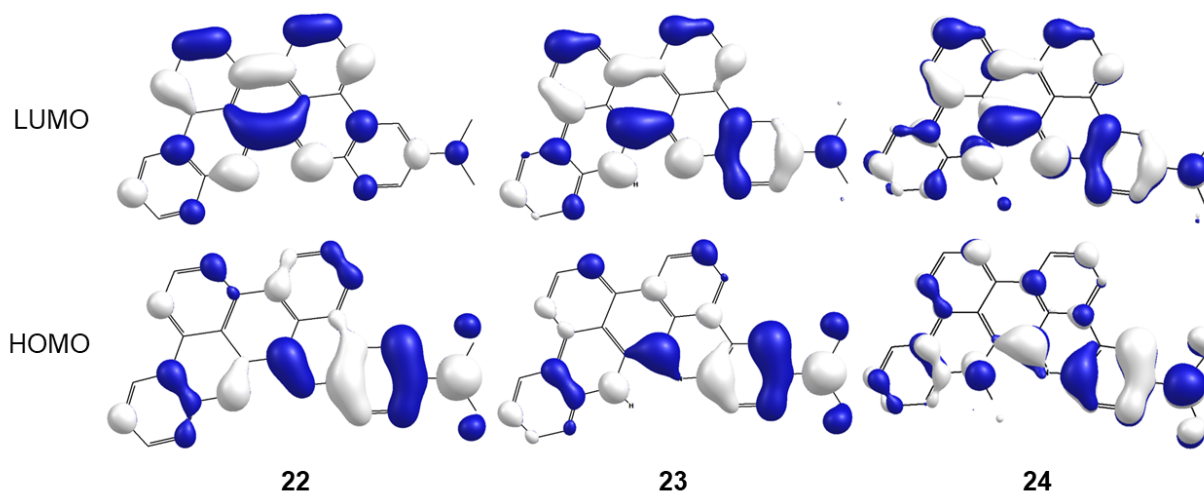


Figure S8. Frontier molecular orbitals of 22-24.

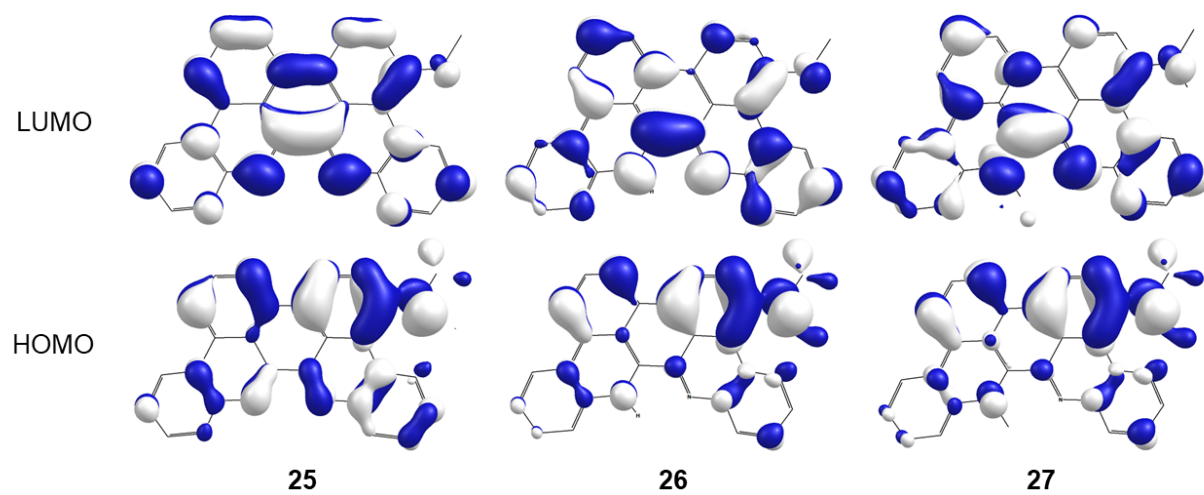


Figure S9. Frontier molecular orbitals of 25-27.

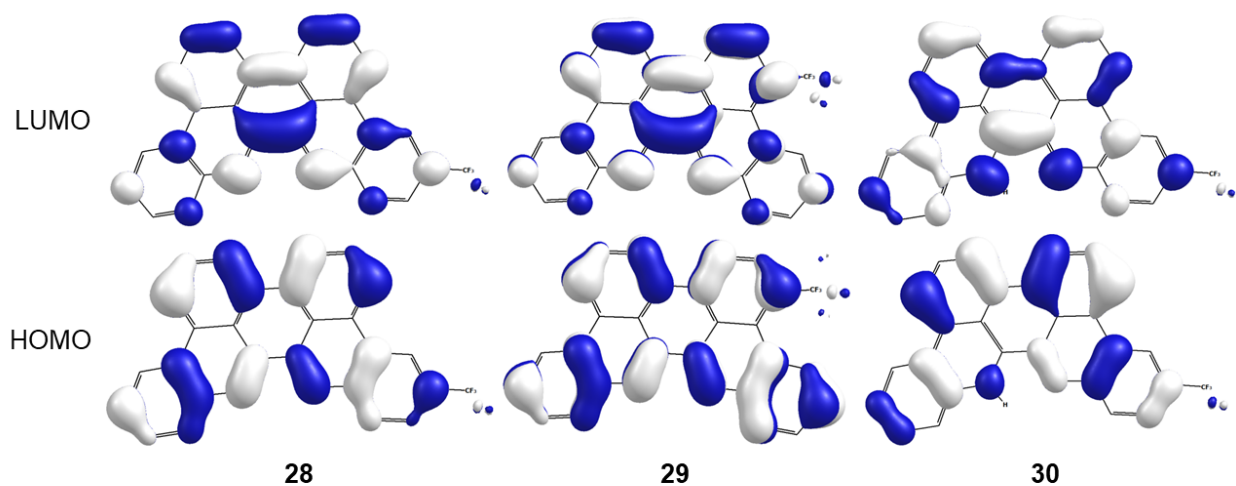


Figure S10. Frontier molecular orbitals of 28-30.

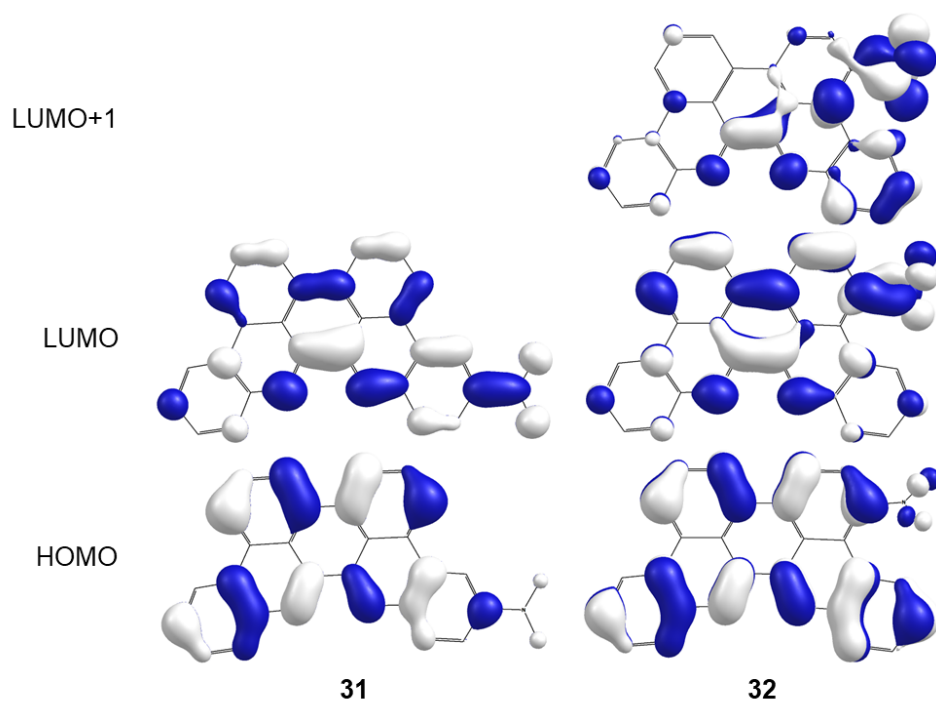


Figure S11. Selected molecular orbitals of 31 and 32.

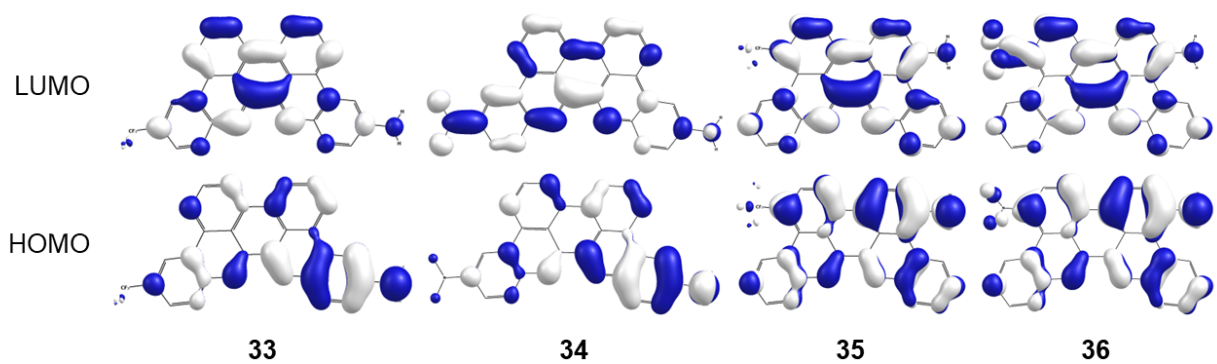


Figure S12. Frontier molecular orbitals of 33-36.

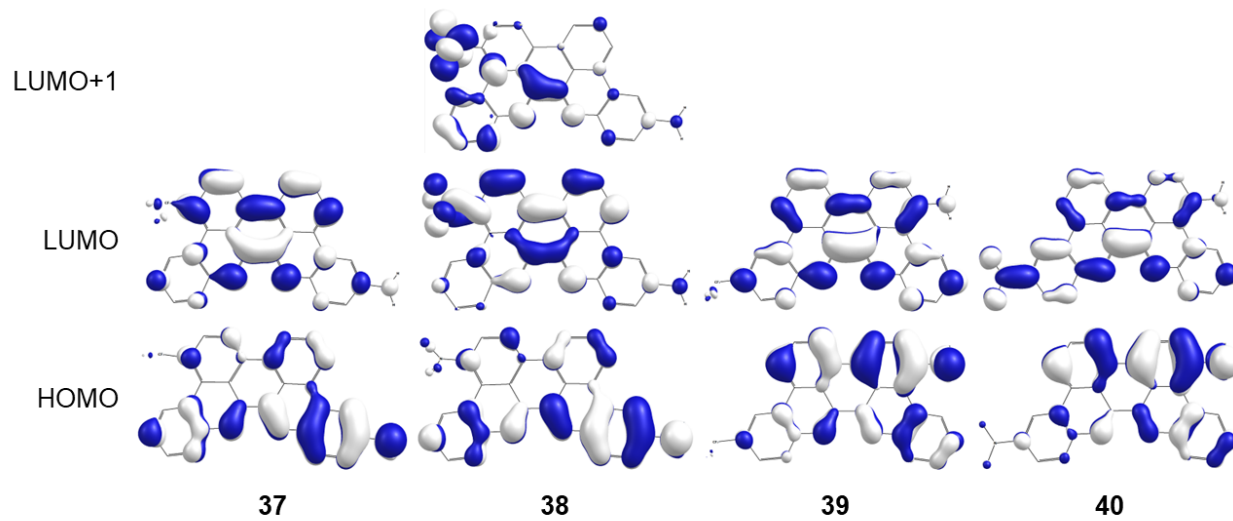


Figure S13. Selected molecular orbitals of 37-40.

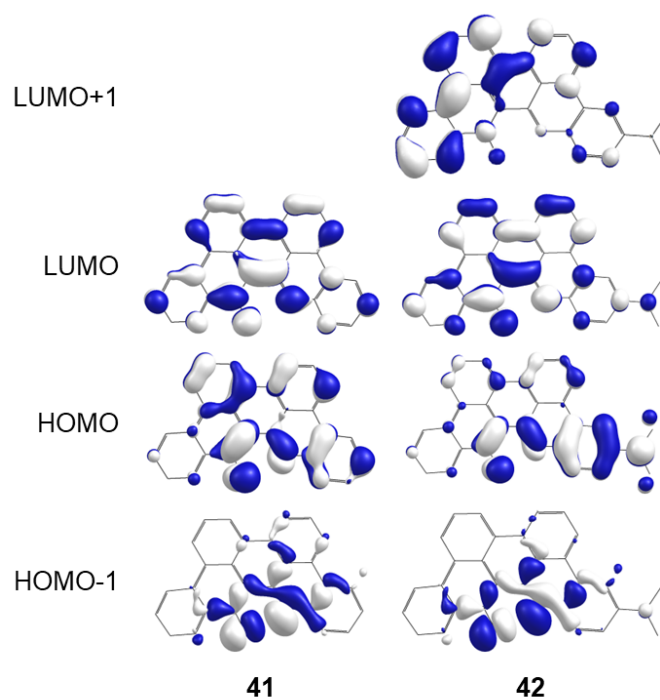


Figure S14. Selected molecular orbitals of 41-42.

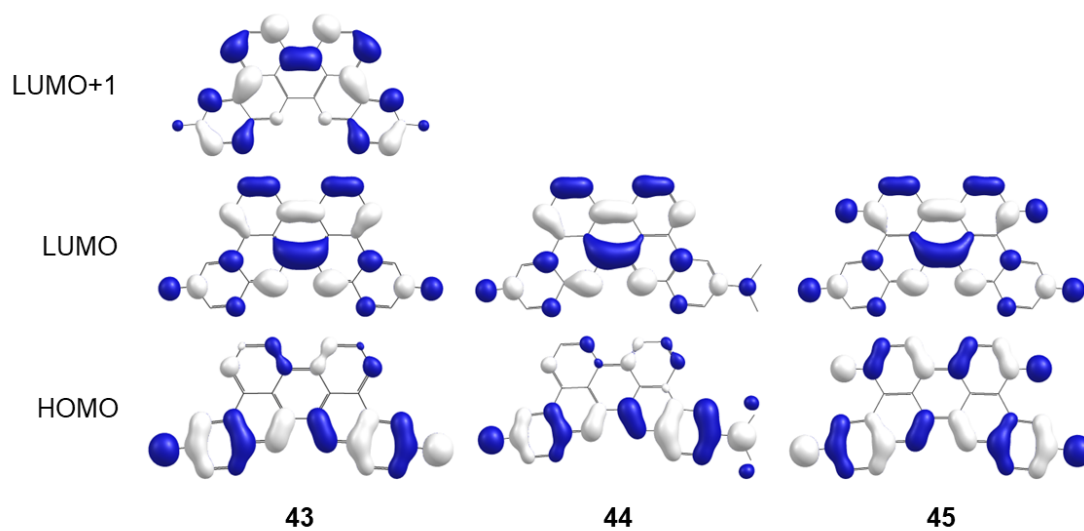


Figure S15. Selected molecular orbitals of 43-45.

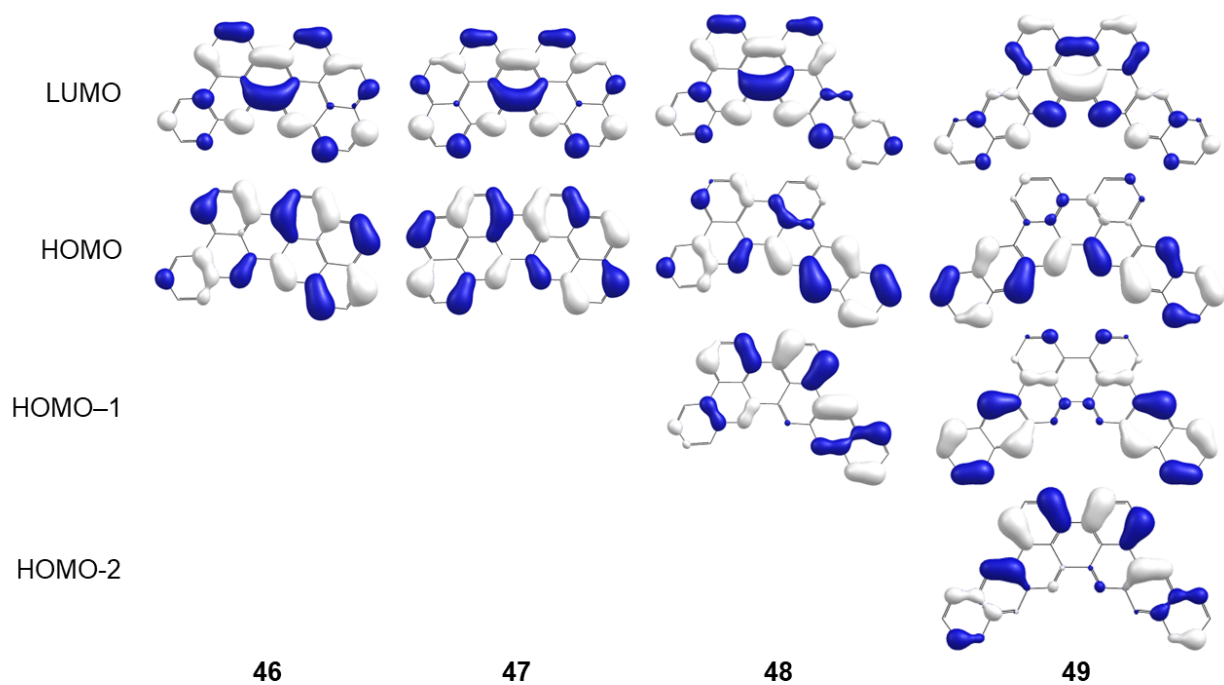


Figure S16. Selected molecular orbitals of 46-49.

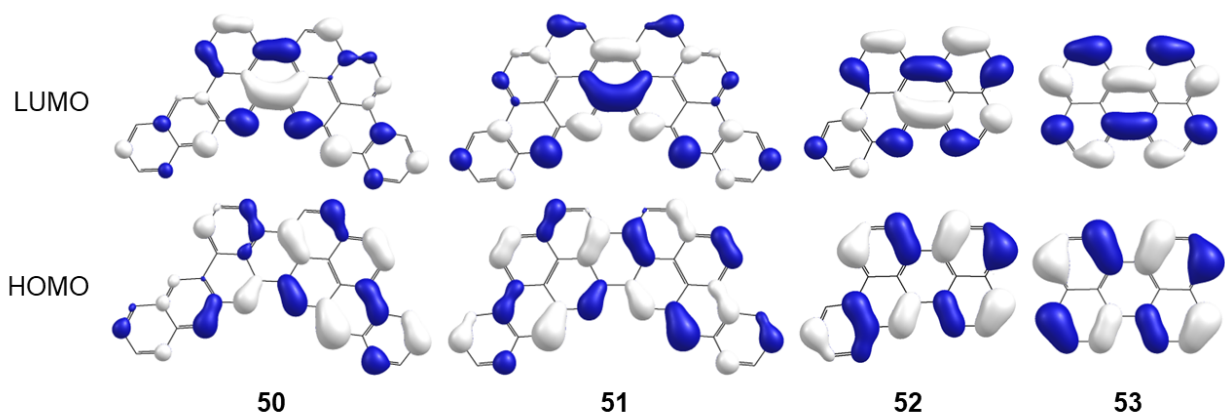


Figure S17. Frontier molecular orbitals of 50-53.

Table S1. TD-DFT vertical excitation energies, oscillator strengths, and MO contributions (>1%) of the two lowest $S_0 \rightarrow S_n$ transitions (TD-RJCOSX-O3LYP/def2-TZVP+def2/J//PBE0-D3(BJ)/def2-SVP).

Structure	S_n	E (eV)	f_{osc}	MO contributions
1	S_1	3.90	0.004	HOMO-1 \rightarrow LUMO (54%), HOMO-1 \rightarrow LUMO+1 (7%), HOMO \rightarrow LUMO (10%), HOMO \rightarrow LUMO+1 (27%)
	S_2	3.99	0.001	HOMO-2 \rightarrow LUMO (99%)
2	S_1	3.49	0.002	HOMO-4 \rightarrow LUMO (17%), HOMO-3 \rightarrow LUMO (60%), HOMO-1 \rightarrow LUMO (20%), HOMO \rightarrow LUMO+1 (1%)
	S_2	3.54	0.196	HOMO-5 \rightarrow LUMO (1%), HOMO-3 \rightarrow LUMO+3 (1%), HOMO-2 \rightarrow LUMO (19%), HOMO-2 \rightarrow LUMO+2 (2%), HOMO \rightarrow LUMO (71%), HOMO \rightarrow LUMO+2 (2%)
3	S_1	2.40	0.021	HOMO-1 \rightarrow LUMO (3%), HOMO \rightarrow LUMO (95%)
	S_2	2.57	0.142	HOMO-2 \rightarrow LUMO (1%), HOMO-1 \rightarrow LUMO (91%), HOMO \rightarrow LUMO (3%)
4	S_1	2.46	0.006	HOMO-1 \rightarrow LUMO (14%), HOMO \rightarrow LUMO (86%)
	S_2	2.50	0.018	HOMO-1 \rightarrow LUMO (85%), HOMO \rightarrow LUMO (14%)
5	S_1	2.88	0.000	HOMO-2 \rightarrow LUMO (99%)
	S_2	2.91	0.571	HOMO-6 \rightarrow LUMO+1 (2%), HOMO-1 \rightarrow LUMO (5%), HOMO \rightarrow LUMO (87%), HOMO \rightarrow LUMO+1 (2%)
6	S_1	2.35	0.252	HOMO-2 \rightarrow LUMO (2%), HOMO-1 \rightarrow LUMO (24%), HOMO \rightarrow LUMO (67%), HOMO \rightarrow LUMO+1 (1%), HOMO \rightarrow LUMO+2 (1%)
	S_2	2.52	0.187	HOMO-3 \rightarrow LUMO (3%), HOMO-2 \rightarrow LUMO (3%), HOMO-1 \rightarrow LUMO (69%), HOMO \rightarrow LUMO (20%)
7	S_1	2.30	0.250	HOMO-4 \rightarrow LUMO (1%), HOMO-2 \rightarrow LUMO (3%), HOMO-1 \rightarrow LUMO (13%), HOMO \rightarrow LUMO (77%)
	S_2	2.50	0.127	HOMO-4 \rightarrow LUMO (5%), HOMO-2 \rightarrow LUMO (4%), HOMO-1 \rightarrow LUMO (78%), HOMO \rightarrow LUMO (9%), HOMO \rightarrow LUMO+2 (1%)
8	S_1	1.96	0.215	HOMO-4 \rightarrow LUMO (4%), HOMO-1 \rightarrow LUMO (7%), HOMO \rightarrow LUMO (85%)
	S_2	2.37	0.070	HOMO-4 \rightarrow LUMO (4%), HOMO-1 \rightarrow LUMO (87%), HOMO \rightarrow LUMO (5%)
9	S_1	1.76	0.192	HOMO-4 \rightarrow LUMO (5%), HOMO-1 \rightarrow LUMO (4%), HOMO \rightarrow LUMO (88%)
	S_2	2.30	0.054	HOMO-5 \rightarrow LUMO (1%), HOMO-4 \rightarrow LUMO (5%), HOMO-1 \rightarrow LUMO (89%), HOMO \rightarrow LUMO (2%)
10	S_1	2.46	0.060	HOMO-1 \rightarrow LUMO (23%), HOMO \rightarrow LUMO (72%)

	S ₂	2.87	0.157	HOMO-2→LUMO (70%), HOMO-1→LUMO (21%), HOMO→LUMO (7%)
11	S ₁	2.64	0.561	HOMO-1→LUMO (4%), HOMO→LUMO (86%), HOMO→LUMO+1 (4%)
	S ₂	2.93	0.000	HOMO-2→LUMO (99%)
12	S ₁	2.46	0.091	HOMO-1→LUMO (17%), HOMO→LUMO (79%)
	S ₂	2.87	0.000	HOMO-2→LUMO (99%)
13	S ₁	2.15	0.155	HOMO-1→LUMO (8%), HOMO→LUMO (89%)
	S ₂	2.89	0.402	HOMO-6→LUMO+1 (1%), HOMO-2→LUMO (3%), HOMO-1→LUMO (71%), HOMO-1→LUMO+1 (1%), HOMO→LUMO (7%), HOMO→LUMO+1 (12%)
14	S ₁	2.62	0.334	HOMO-1→LUMO (7%), HOMO→LUMO (85%), HOMO→LUMO+1 (3%)
	S ₂	2.91	0.003	HOMO-3→LUMO (8%), HOMO-2→LUMO (90%)
15	S ₁	2.75	0.283	HOMO-1→LUMO (8%), HOMO→LUMO (85%)
	S ₂	2.90	0.000	HOMO-2→LUMO (99%)
16	S ₁	2.51	0.345	HOMO-1→LUMO (5%), HOMO→LUMO (86%), HOMO→LUMO+1 (3%)
	S ₂	2.91	0.006	HOMO-3→LUMO (5%), HOMO-2→LUMO (90%), HOMO-1→LUMO (4%)
17	S ₁	2.59	0.573	HOMO-6→LUMO+1 (1%), HOMO-1→LUMO (7%), HOMO-1→LUMO+3 (1%), HOMO→LUMO (84%), HOMO→LUMO+1 (2%)
	S ₂	2.87	0.163	HOMO-3→LUMO (1%), HOMO-2→LUMO (3%), HOMO-1→LUMO (58%), HOMO→LUMO (8%), HOMO→LUMO+1 (26%)
18	S ₁	2.43	0.888	HOMO-3→LUMO (2%), HOMO-3→LUMO+1 (1%), HOMO-2→LUMO (2%), HOMO-1→LUMO (1%), HOMO-1→LUMO+3 (1%), HOMO→LUMO (87%)
	S ₂	2.51	0.037	HOMO-1→LUMO (91%), HOMO→LUMO (1%), HOMO→LUMO+2 (2%)
19	S ₁	1.83	0.242	HOMO-3→LUMO (2%), HOMO-1→LUMO (1%), HOMO→LUMO (91%)
	S ₂	2.67	0.069	HOMO-4→LUMO (1%), HOMO-3→LUMO (8%), HOMO-1→LUMO (83%), HOMO→LUMO+2 (2%)
20	S ₁	2.41	0.542	HOMO-2→LUMO (3%), HOMO-1→LUMO (37%), HOMO-1→LUMO+3 (1%), HOMO→LUMO (53%)
	S ₂	2.51	0.349	HOMO-3→LUMO (2%), HOMO-2→LUMO (1%), HOMO-1→LUMO (56%), HOMO→LUMO (32%), HOMO→LUMO+2 (2%)

21	S ₁	1.83	0.238	HOMO-3→LUMO (2%), HOMO→LUMO (92%), HOMO→LUMO+3 (1%)
	S ₂	2.62	0.063	HOMO-5→LUMO (5%), HOMO-3→LUMO (6%), HOMO-1→LUMO (83%), HOMO→LUMO+2 (2%)
22	S ₁	2.46	0.552	HOMO-1→LUMO (4%), HOMO→LUMO (87%), HOMO→LUMO+1 (4%)
	S ₂	2.92	0.000	HOMO-2→LUMO (99%)
23	S ₁	2.30	0.951	HOMO-2→LUMO (2%), HOMO-1→LUMO (4%), HOMO→LUMO (85%)
	S ₂	2.48	0.163	HOMO-1→LUMO (89%), HOMO-1→LUMO+1 (1%), HOMO→LUMO (4%)
24	S ₁	2.35	1.048	HOMO-2→LUMO (3%), HOMO-1→LUMO+3 (1%), HOMO→LUMO (88%)
	S ₂	2.42	0.058	HOMO-1→LUMO (93%), HOMO-1→LUMO+1 (1%), HOMO→LUMO+2 (1%)
25	S ₁	2.46	0.303	HOMO-1→LUMO (8%), HOMO→LUMO (84%), HOMO→LUMO+1 (4%)
	S ₂	2.91	0.026	HOMO-3→LUMO (11%), HOMO-2→LUMO (78%), HOMO-1→LUMO (9%), HOMO→LUMO (1%)
26	S ₁	1.74	0.256	HOMO-1→LUMO (1%), HOMO→LUMO (92%), HOMO→LUMO+1 (1%)
	S ₂	2.60	0.091	HOMO-4→LUMO (1%), HOMO-3→LUMO (4%), HOMO-2→LUMO (10%), HOMO-1→LUMO (77%), HOMO→LUMO+2 (1%)
27	S ₁	1.76	0.263	HOMO-3→LUMO (1%), HOMO→LUMO (92%), HOMO→LUMO+1 (1%)
	S ₂	2.57	0.087	HOMO-5→LUMO (5%), HOMO-3→LUMO (5%), HOMO-2→LUMO (3%), HOMO-1→LUMO (82%), HOMO→LUMO+2 (1%)
28	S ₁	2.86	0.000	HOMO-2→LUMO (99%)
	S ₂	2.87	0.545	HOMO-5→LUMO+1 (1%), HOMO-1→LUMO (6%), HOMO→LUMO (84%), HOMO→LUMO+1 (3%)
29	S ₁	2.80	0.006	HOMO-3→LUMO (3%), HOMO-2→LUMO (70%), HOMO-1→LUMO (25%)
	S ₂	2.86	0.574	HOMO-6→LUMO+1 (2%), HOMO-1→LUMO (4%), HOMO→LUMO (87%), HOMO→LUMO+1 (2%)
30	S ₁	2.34	0.317	HOMO-4→LUMO (1%), HOMO-3→LUMO (2%), HOMO-2→LUMO (2%), HOMO-1→LUMO (8%), HOMO→LUMO (82%), HOMO→LUMO+1 (1%)

	S ₂	2.59	0.105	HOMO-3→LUMO (2%), HOMO-2→LUMO (2%), HOMO-1→LUMO (85%), HOMO→LUMO (6%), HOMO→LUMO+2 (1%)
31	S ₁	2.65	0.510	HOMO-1→LUMO (4%), HOMO→LUMO (85%), HOMO→LUMO+1 (5%)
	S ₂	2.74	0.000	HOMO-2→LUMO (98%)
32	S ₁	2.66	0.337	HOMO-3→LUMO (1%), HOMO-1→LUMO (6%), HOMO→LUMO (70%), HOMO→LUMO+1 (19%)
	S ₂	2.76	0.003	HOMO-3→LUMO (2%), HOMO-2→LUMO (90%), HOMO-2→LUMO+1 (2%), HOMO-1→LUMO (4%)
33	S ₁	2.61	0.616	HOMO-1→LUMO (4%), HOMO→LUMO (87%), HOMO→LUMO+1 (3%)
	S ₂	2.91	0.000	HOMO-2→LUMO (99%)
34	S ₁	2.45	0.748	HOMO→LUMO (90%), HOMO→LUMO+1 (3%), HOMO→LUMO+2 (1%)
	S ₂	2.78	0.000	HOMO-2→LUMO (98%)
35	S ₁	2.56	0.410	HOMO-1→LUMO (5%), HOMO→LUMO (85%), HOMO→LUMO+1 (4%)
	S ₂	2.86	0.006	HOMO-3→LUMO (8%), HOMO-2→LUMO (90%)
36	S ₁	2.51	0.530	HOMO-1→LUMO (2%), HOMO-1→LUMO+1 (1%), HOMO→LUMO (88%), HOMO→LUMO+1 (1%), HOMO→LUMO+2 (1%)
	S ₂	2.66	0.039	HOMO-3→LUMO (1%), HOMO-1→LUMO (11%), HOMO→LUMO (2%), HOMO→LUMO+1 (83%)
37	S ₁	2.49	0.467	HOMO-1→LUMO (3%), HOMO→LUMO (86%), HOMO→LUMO+1 (6%), HOMO→LUMO+3 (1%)
	S ₂	2.85	0.001	HOMO-3→LUMO (9%), HOMO-2→LUMO (88%), HOMO-1→LUMO (2%)
38	S ₁	2.26	0.280	HOMO-1→LUMO (2%), HOMO→LUMO (81%), HOMO→LUMO+1 (14%)
	S ₂	2.76	0.244	HOMO-3→LUMO (2%), HOMO-2→LUMO (15%), HOMO-1→LUMO (1%), HOMO→LUMO (9%), HOMO→LUMO+1 (65%), HOMO→LUMO+2 (1%)
39	S ₁	2.44	0.332	HOMO-1→LUMO (4%), HOMO→LUMO (88%), HOMO→LUMO+1 (3%)
	S ₂	2.89	0.007	HOMO-2→LUMO (87%), HOMO-1→LUMO (12%)
40	S ₁	2.20	0.309	HOMO-1→LUMO (3%), HOMO→LUMO (90%), HOMO→LUMO+1 (3%)
	S ₂	2.76	0.003	HOMO-2→LUMO (83%), HOMO-1→LUMO (14%), HOMO→LUMO+1 (1%)

41	S ₁	2.24	0.008	HOMO-1→LUMO (84%), HOMO→LUMO (14%)
	S ₂	2.84	0.004	HOMO-2→LUMO (25%), HOMO→LUMO+1 (73%)
42	S ₁	2.26	0.060	HOMO-2→LUMO (3%), HOMO-1→LUMO (75%), HOMO→LUMO (19%)
	S ₂	2.47	0.326	HOMO-2→LUMO (6%), HOMO-1→LUMO (19%), HOMO→LUMO (43%), HOMO→LUMO+1 (28%)
43	S ₁	2.49	0.622	HOMO-7→LUMO+1 (1%), HOMO-2→LUMO (1%), HOMO→LUMO (75%), HOMO→LUMO+1 (15%), HOMO→LUMO+3 (4%)
	S ₂	2.81	0.230	HOMO-7→LUMO (2%), HOMO-2→LUMO (22%), HOMO→LUMO (12%), HOMO→LUMO+1 (59%), HOMO→LUMO+3 (2%)
44	S ₁	2.35	0.652	HOMO-2→LUMO (2%), HOMO-1→LUMO (3%), HOMO→LUMO (82%), HOMO→LUMO+1 (8%), HOMO→LUMO+3 (1%)
	S ₂	2.71	0.053	HOMO-7→LUMO (2%), HOMO-2→LUMO (4%), HOMO-1→LUMO (32%), HOMO→LUMO (2%), HOMO→LUMO+1 (56%), HOMO→LUMO+2 (2%)
45	S ₁	2.21	0.657	HOMO-9→LUMO+1 (1%), HOMO-1→LUMO (4%), HOMO-1→LUMO+1 (5%), HOMO-1→LUMO+3 (4%), HOMO→LUMO (73%), HOMO→LUMO+1 (7%), HOMO→LUMO+3 (2%)
	S ₂	2.27	0.089	HOMO-1→LUMO (52%), HOMO-1→LUMO+1 (2%), HOMO→LUMO (9%), HOMO→LUMO+1 (35%)
46	S ₁	2.65	0.583	HOMO-6→LUMO (1%), HOMO-1→LUMO (1%), HOMO→LUMO (87%), HOMO→LUMO+1 (2%), HOMO→LUMO+2 (2%)
	S ₂	2.80	0.000	HOMO-3→LUMO (99%)
47	S ₁	2.43	0.680	HOMO-6→LUMO (3%), HOMO-6→LUMO+3 (1%), HOMO-3→LUMO (2%), HOMO-3→LUMO+2 (2%), HOMO→LUMO (89%)
	S ₂	2.74	0.000	HOMO-2→LUMO (99%)
48	S ₁	2.52	0.083	HOMO-1→LUMO (40%), HOMO→LUMO (48%), HOMO→LUMO+1 (8%)
	S ₂	2.81	0.627	HOMO-3→LUMO (1%), HOMO-1→LUMO (43%), HOMO→LUMO (45%), HOMO→LUMO+1 (5%)
49	S ₁	2.45	0.128	HOMO-2→LUMO (30%), HOMO→LUMO (61%), HOMO→LUMO+1 (6%)
	S ₂	2.51	0.046	HOMO-1→LUMO (90%), HOMO→LUMO+2 (7%)

50	S₁	2.34	0.089	HOMO-2→LUMO (1%), HOMO-1→LUMO (79%), HOMO→LUMO (10%), HOMO→LUMO+1 (7%)
	S₂	2.36	0.492	HOMO-2→LUMO (2%), HOMO-1→LUMO (8%), HOMO→LUMO (76%), HOMO→LUMO+1 (6%), HOMO→LUMO+2 (1%)
51	S₁	2.17	0.728	HOMO-5→LUMO (3%), HOMO-2→LUMO (1%), HOMO→LUMO (90%)
	S₂	2.35	0.045	HOMO-1→LUMO (80%), HOMO→LUMO+1 (18%)
52	S₁	2.85	0.000	HOMO-1→LUMO (99%)
	S₂	2.96	0.549	HOMO-5→LUMO+1 (1%), HOMO-4→LUMO+1 (1%), HOMO-2→LUMO (3%), HOMO→LUMO (89%), HOMO→LUMO+1 (1%)
53	S₁	2.82	0.000	HOMO-1→LUMO (99%)
	S₂	3.19	0.001	HOMO-2→LUMO (99%)

Table S2. Selected bond lengths of ground-state optimized geometries in vacuum (PBE0-D3(BJ)/def2-SVP).

Structure	Bond length (Å)			
	C(6)-C(6')	C(7)-C(7')	N(5)-C(6)	N(5')-C(6')
1	<i>n/a</i>	<i>n/a</i>	<i>n/a</i>	<i>n/a</i>
2	1.497	<i>n/a</i>	1.299	1.299
3	1.488	<i>n/a</i>	1.322	1.304
4	1.497	<i>n/a</i>	1.328	1.296
5	1.483	1.473	1.302	1.302
6	1.456	1.471	1.322	1.307
7	1.470	1.464	1.345	1.310
8	1.405	1.484	1.327	1.327
9	1.472	1.460	1.344	1.344
10	1.483	1.473	1.300	1.302
11	1.480	1.473	1.305	1.303
12	1.484	1.473	1.302	1.302
13	1.477	1.473	1.304	1.304
14	1.480	1.471	1.303	1.303
15	1.483	1.474	1.304	1.302
16	1.484	1.468	1.301	1.303
17	1.481	1.468	1.303	1.304
18	1.443	1.470	1.317	1.327
19	1.456	1.460	1.307	1.325
20	1.455	1.463	1.320	1.350
21	1.470	1.454	1.309	1.348
22	1.479	1.473	1.305	1.303
23	1.441	1.470	1.318	1.328
24	1.453	1.463	1.322	1.352
25	1.484	1.469	1.301	1.302
26	1.455	1.460	1.308	1.326
27	1.468	1.454	1.310	1.348
28	1.483	1.473	1.303	1.302

29	1.484	1.472	1.299	1.302
30	1.458	1.471	1.307	1.322
31	1.482	1.472	1.304	1.302
32	1.482	1.472	1.300	1.302
33	1.478	1.473	1.305	1.304
34	1.477	1.472	1.306	1.305
35	1.485	1.466	1.301	1.300
36	1.484	1.465	1.301	1.301
37	1.480	1.472	1.305	1.300
38	1.478	1.472	1.305	1.301
39	1.484	1.467	1.301	1.304
40	1.484	1.467	1.301	1.305
41	1.469	1.466	1.363	1.306
42	1.467	1.467	1.308	1.362
43	1.475	1.472	1.308	1.308
44	1.475	1.472	1.306	1.308
45	1.473	1.452	1.307	1.307
46	1.482	1.468	1.304	1.303
47	1.482	1.463	1.305	1.305
48	1.483	1.473	1.298	1.302
49	1.483	1.473	1.298	1.298
50	1.482	1.468	1.300	1.299
51	1.481	1.463	1.301	1.301
52	1.480	1.471	1.302	1.319
53	1.478	1.470	1.318	1.318

Table S3. Selected dihedral angles of ground-state optimized geometries in vacuum (PBE0-D3(BJ)/def2-SVP).

Structure	Dihedral angle (°)		
	N(5)-C(6)-C(6')-N(5')	C(1)-C-C-C(10)	C(1')-C-C-C(10')
1	<i>n/a</i>	0.0	<i>n/a</i>
2	128.3	1.5	1.5
3	40.1	2.9	3.8
4	77.2	1.0	0.6
5	0.1	0.0	0.0
6	0.0	0.0	0.0
7	16.4	7.3	0.7
8	0.0	0.0	0.0
9	13.8	1.1	1.1
10	3.6	13.1	0.3
11	0.1	0.3	0.0
12	0.1	0.1	0.0
13	0.5	0.7	0.1
14	7.1	3.2	3.9
15	0.1	0.4	0.0
16	0.5	14.6	0.5
17	0.3	14.3	0.5
18	0.0	0.0	0.0
19	0.1	13.9	0.4
20	15.7	0.7	7.8
21	16.9	12.7	6.9
22	0.0	0.1	0.0
23	0.0	0.0	0.0
24	15.6	0.8	7.8
25	4.0	11.7	0.7
26	2.0	12.3	0.8
27	18.8	11.3	6.4
28	0.0	0.0	0.0

29	1.1	15.9	0.7
30	0.0	0.0	0.0
31	0.0	0.0	0.0
32	0.5	11.4	0.3
33	0.1	0.4	0.1
34	0.0	0.3	0.0
35	1.4	14.8	15.7
36	1.1	14.9	11.6
37	1.0	0.3	16.1
38	0.3	0.0	11.5
39	0.6	14.6	0.5
40	0.6	14.6	0.5
41	7.7	1.2	0.1
42	7.4	0.0	1.2
43	0.1	0.0	0.0
44	0.0	0.1	0.0
45	0.0	0.0	0.0
46	0.0	0.0	0.0
47	0.0	0.0	0.0
48	0.1	0.0	0.0
49	0.0	0.0	0.0
50	0.0	0.0	0.0
51	0.0	0.0	0.0
52	0.1	0.0	<i>n/a</i>
53	0.0	<i>n/a</i>	<i>n/a</i>

Optimized Coordinates

phenanthridine (**1**), S_{0,eq} in vacuum

C	-5.09986583926026	-1.83074983015548	0.00067432251525
C	-3.72100856040356	-1.79070624143723	-0.00042903779992
C	-3.03445245365827	-0.55757352400766	0.00112256447480
C	-3.77448567276231	0.65715345530750	0.00385260218750
C	-5.18340648130055	0.58656249262277	0.00493012095861
C	-5.83484078807062	-0.63172711492419	0.00337579309426
C	-3.03402952880264	1.90095852245046	0.00537284355838
C	-1.61897132338032	1.81987291593571	0.00403301074153
C	-1.01059468681280	0.51865758384889	0.00126813149918
C	-0.83980276322494	2.99468802117031	0.00540199668223
H	0.24991472287582	2.90597267920503	0.00432495476899
C	-1.44593123420938	4.23419585526430	0.00805735282738
C	-2.85020819179006	4.32126189220700	0.00939707581441
C	-3.62945427270391	3.18011275953034	0.00808580904382
H	-5.62180864923366	-2.79042764610807	-0.00054339906654
H	-3.11467314152024	-2.69825379359743	-0.00251480837167
H	-5.77225742447656	1.50534256321198	0.00702196133755
H	-6.92682274750848	-0.66243793474909	0.00425269497834
H	0.08711555540398	0.46293906944478	0.00024108678806
H	-0.84260683516567	5.14462467961288	0.00911907448160
H	-3.33092970164771	5.30242378353375	0.01149867646774
H	-4.71602983136502	3.27642579356568	0.00917060597988
N	-1.66125015098279	-0.59861598193224	-0.00011343296138

biphe (**2**), S_{0,eq} in vacuum

N	1.34812610907975	-1.00732274895384	0.02452302163207
C	1.45422464615899	1.40699258773564	0.14573486719507
C	0.74615538826436	0.14155228877286	0.10360888145247
C	3.52987171770222	0.09375876311331	-0.05797500120981
C	0.79531783997932	2.64764875830686	0.29649720718730

C	2.87262101648395	1.37712229739583	0.06666113589219
C	2.71173895645042	-1.06546361817037	-0.06303683414978
C	3.58061689167951	2.59653120850620	0.12622543424450
H	4.66945671144805	2.59423390358093	0.06640783770606
C	4.92688594284114	-0.07162885149663	-0.16293306309961
H	5.57986131931035	0.80233659311901	-0.16619264706451
C	1.51344182524575	3.82378127645739	0.35873665964879
H	0.99113341847602	4.77572049456670	0.47678851517364
C	4.67291169230731	-2.47650799008932	-0.26476086076541
H	5.12496995879772	-3.46767052069253	-0.34590613495399
C	3.30387016261163	-2.34329667315189	-0.16585887414520
H	2.63471344798533	-3.20564478367459	-0.16849711917495
C	5.48819051907907	-1.33017366245509	-0.26450493000900
H	6.57262954382057	-1.43399084493369	-0.34592702408181
C	2.91527858585374	3.79718990757567	0.26758647044307
H	3.48275886771268	4.72975757285046	0.31323785733856
N	-1.34522079332350	0.85363723228922	-0.75341443177840
C	-1.46505941919992	-0.78853335682894	1.01965684859421
C	-0.75011907827037	0.09039680261701	0.11367069472842
C	-3.53135430328314	-0.00191547289437	-0.06944037668427
C	-0.81444317465707	-1.56723367734086	2.00271607522593
C	-2.88221551231684	-0.82928637746609	0.92481708875351
C	-2.70735459201365	0.82736871048514	-0.87342840684119
C	-3.59713158445646	-1.66312323891147	1.81097116715991
H	-4.68512039388193	-1.70864168126535	1.75314259142731
C	-4.92609550774644	0.03618026449637	-0.27723383887743
H	-5.58358354988607	-0.59405623188155	0.32334192620975
C	-1.53931192771613	-2.36832531768363	2.86043441155082
H	-1.02329251413061	-2.96401855191805	3.61660893969329
C	-4.65863126228269	1.68558644042181	-2.02835705469164
H	-5.10465946405951	2.33522391928984	-2.78490601366107
C	-3.29161831891344	1.66618251828628	-1.84763970565761
H	-2.61795842499933	2.28410869432983	-2.44410551231407

C	-5.47966559245761	0.86222923610867	-1.23669801341518
H	-6.56249604784937	0.87413821733026	-1.38074977808017
C	-2.93975943777156	-2.41977935903774	2.75941865812398
H	-3.51263409279407	-3.05752017111772	3.43684055191193
H	0.27184142969679	-1.53858035858074	2.06655624230439
H	-0.29179099897498	2.66623580090912	0.34898253705791

biphe (2), T_{1,eq} in vacuum

N	1.26801757944827	-0.82627893374636	0.53579782894183
C	1.41477604465125	1.53308357181488	-0.07704236719271
C	0.65198401655263	0.35522523859457	0.37689444555911
C	3.45721717978390	0.12503629788964	0.07141153297232
C	0.83315958361319	2.78186678817410	-0.37190075742523
C	2.82764111368823	1.40531349958521	-0.20332214666043
C	2.59668972229267	-0.95975971830950	0.41588398799098
C	3.58384981736309	2.52262508827567	-0.60628251064056
H	4.66565873523740	2.43012200888721	-0.70625429088283
C	4.83755535915579	-0.11633969776994	-0.01507569212739
H	5.51853090984411	0.69554628166538	-0.27451066894240
C	1.59952857350357	3.86704873010256	-0.76232072779787
H	1.11383874167446	4.82128068802449	-0.97923351297674
C	4.51455154784573	-2.45291259987430	0.54574147802867
H	4.93504479462517	-3.44550159410182	0.72348816138795
C	3.15564256400383	-2.24912374983999	0.63626949377123
H	2.46327047896868	-3.05627804229494	0.88262005316241
C	5.36352042129950	-1.37790059171064	0.22214056864320
H	6.44196292987413	-1.53621718211109	0.15173791633929
C	2.98635969119972	3.73823644661702	-0.88335661745327
H	3.59674836243404	4.58820209324226	-1.19739223225586
N	-1.52802032025565	1.45472908104321	0.41433405923582
C	-1.42642611115535	-0.83324502384765	1.20123981353956
C	-0.73909293030436	0.35395535364493	0.68649242886899
C	-3.40984019383071	-0.00097173413795	-0.03251505681875

C	-0.83756256045413	-1.76568621172765	2.06711626081727
C	-2.75984307867302	-1.04621040322718	0.76290947864092
C	-2.75642678626339	1.28550618282869	-0.05411515713527
C	-3.42583705241243	-2.21381635063948	1.14908734625995
H	-4.44899642895677	-2.39067745315945	0.81309559144036
C	-4.66521345009119	-0.11791327465309	-0.62088109377258
H	-5.17515525004252	-1.08313450979111	-0.62570228054298
C	-1.52236524703152	-2.91747805688817	2.44793532227121
H	-1.04727669235961	-3.62883416090995	3.12727765038375
C	-4.70782787722914	2.25847754320646	-1.14492445145489
H	-5.22701430734344	3.12014174415426	-1.57030606972457
C	-3.46752734273963	2.41536947709192	-0.56517521266792
H	-2.97026840780145	3.38613845044576	-0.52395344248780
C	-5.30346587374087	0.98594929826051	-1.19408499324935
H	-6.28248296174086	0.85982803845110	-1.66128219385652
C	-2.81109364153610	-3.15191598296912	1.97596993687966
H	-3.35214624800008	-4.05415026399340	2.26975257530425
H	0.16204127595515	-1.57291606897596	2.44987493684896
H	-0.24660668105232	2.87877970267876	-0.27583939122177

[biphe-H]⁺ (**3**), S_{0,eq} in vacuum

N	1.30530099183611	-0.34506669262693	-1.10156505393097
C	1.53290996424064	0.58073631489100	1.06382370862708
C	0.72343419280306	0.03937090983060	0.02151244321451
C	3.53088455468868	0.05112682451569	-0.31601639469353
C	0.95307289566680	1.19770222885185	2.20008729103244
C	2.95387643553062	0.56523381292998	0.90819097231397
C	2.65777096356304	-0.36724271858959	-1.34582065959575
C	3.74031419490335	1.10026655011072	1.94681240301137
H	4.82693467087049	1.09271526905621	1.86641697726714
C	4.91519439410018	-0.02405925324734	-0.57325203692895
H	5.62812715301747	0.28112336534072	0.19246913252118
C	1.75255259317377	1.73137846729107	3.18452496627317

H	1.30176339587920	2.21381282212159	4.05359425965501
C	4.49549816276565	-0.87500927280633	-2.80262388915061
H	4.88020514328692	-1.22909986431053	-3.76089632285146
C	3.13394600575359	-0.82287723460748	-2.58554838091767
H	2.42737154548764	-1.13593556841621	-3.35771999223938
C	5.38677159901462	-0.47842713235482	-1.78955628029906
H	6.46274097340200	-0.52816459762546	-1.96697555906601
C	3.15278486349292	1.66196487272478	3.06339532030497
H	3.78464666377944	2.07685534151588	3.85187252571711
N	-1.26198535272240	0.29870052549765	-1.15037313907824
C	-1.54137267488018	-0.60874265252959	1.08067922069494
C	-0.76031620547046	-0.06828584356910	-0.00423326024434
C	-3.51410283679717	-0.06157891661240	-0.30000165374989
C	-0.97459936161759	-1.23130846824041	2.21758792627383
C	-2.95682570554509	-0.57781294949847	0.92998410672966
C	-2.61170194257449	0.32187150976688	-1.33194881502121
C	-3.75393355897767	-1.10112163873125	1.97111347666338
H	-4.84022268001847	-1.07993987081938	1.88445891313974
C	-4.89655705480736	0.04383833807729	-0.55433747658749
H	-5.61786265695737	-0.22982670585310	0.21609591863283
C	-1.78010672867360	-1.75058199295506	3.20750505278604
H	-1.33277494171557	-2.23571462812973	4.07725884348044
C	-4.45937164480307	0.85204062465430	-2.79990012170306
H	-4.84072950903771	1.20267788100033	-3.76100354097014
C	-3.10254007251436	0.77070262649627	-2.57870570540210
H	-2.37558297258440	1.05803981881399	-3.34014734179076
C	-5.35795525239750	0.49129677194093	-1.77738086772940
H	-6.43336006353741	0.56542308873407	-1.95255159626076
C	-3.17938181091871	-1.66604599001168	3.09043661126034
H	-3.81555548892418	-2.07096584881558	3.88030973110981
H	0.10861271639611	-1.31953066320721	2.30844069901603
H	-0.13158981159469	1.26084325070550	2.28318630619011
H	0.65221425341717	-0.58448271130966	-1.85339871770432

[biphe-Me]⁺ (4), S_{0,eq} in vacuum

N	1.37868679935937	-0.74737455298329	0.25809972369298
C	1.36102008045775	1.32904888252590	-1.00030296828201
C	0.74523338109550	0.20675737047790	-0.34785054848180
C	3.49858657929832	0.35050944029632	-0.27013001727870
C	0.61541813562844	2.32337488485021	-1.67218748479378
C	2.77963054473898	1.39965530764643	-0.96013322536384
C	2.74597363660671	-0.70402698324508	0.31999203607914
C	3.40762892729517	2.48919638895425	-1.60093368114644
H	4.49442352855218	2.57444507138357	-1.58899815332360
C	4.90338194314363	0.31061957243523	-0.15441863421754
H	5.51089348048409	1.10246764252265	-0.59394026434547
C	1.25871996378583	3.37423082555582	-2.29015137697913
H	0.68303314387093	4.14301348811133	-2.80926679376247
C	4.77838879425028	-1.76375104937220	1.09361217678132
H	5.28664140129754	-2.57483181339826	1.61908694993172
C	3.40336716329406	-1.75285960560550	0.99772656459027
H	2.78618601463837	-2.53834834778918	1.43692080661766
C	5.52911201069775	-0.72435543871616	0.51348031862574
H	6.61833922397725	-0.73466330437018	0.59182308369758
C	2.66335109606763	3.45410666118766	-2.24989666880371
H	3.17074772192730	4.28824785767302	-2.73927484021900
N	-1.33537144392410	-0.79754336115043	-1.11657332100573
C	-1.49657474959745	0.83926118137672	0.62814792109042
C	-0.74494638390969	0.07297814219929	-0.30555132709834
C	-3.52411003681940	-0.29625201202309	-0.17493328483394
C	-0.84079974812804	1.75430794538433	1.48916991124337
C	-2.90760515694193	0.68391624655972	0.68871046112183
C	-2.71433746234202	-1.04442860071039	-1.06454100155309
C	-3.62700415575254	1.47765249613828	1.60190421750850
H	-4.71056297342923	1.38959183718524	1.67299278639577
C	-4.90978906435559	-0.55668308926039	-0.16110157816268

H	-5.55455290451062	0.00642364454566	0.51278674037954
C	-1.57153205867365	2.51282749590127	2.37460664334113
H	-1.06818183116093	3.21755787156563	3.03878044114803
C	-4.65133144990026	-2.26124709888553	-1.84133906928485
H	-5.08645533824512	-3.03117733457119	-2.48134918494842
C	-3.29013725993816	-2.02995781103845	-1.88762631752946
H	-2.67882964085935	-2.62778084264940	-2.55980653190204
C	-5.46832128321255	-1.51765612663008	-0.97826164158896
H	-6.54363216748743	-1.70245858311686	-0.94721144802818
C	-2.97115144119431	2.37444980500418	2.42357174038975
H	-3.54870828789502	2.97967477326583	3.12590032063957
H	0.24455533935303	1.85075857181325	1.44599810485544
H	-0.47540216956835	2.26027513808635	-1.69930416799677
C	-0.54519356827333	-1.53680691130276	-2.10383612621267
H	-1.01731043321988	-1.43929921859632	-3.08829231462530
H	0.46454433789726	-1.12458551855750	-2.14891365522120
H	-0.48462223837840	-2.59476093867382	-1.81628532114063

[biphe-Me]⁺ (4), S_{0,eq} in chloroform

N	1.39969181814598	-0.67230841351403	0.41329315673288
C	1.35042733548360	1.23401646439066	-1.08646837174577
C	0.75048179268499	0.18155741109513	-0.31215247939692
C	3.50370535402608	0.38810014501562	-0.24927165983074
C	0.58383032336249	2.13348563673083	-1.85927021013917
C	2.76621334257612	1.33946369005393	-1.05378914426980
C	2.76830592350834	-0.59930348555125	0.46291168254224
C	3.37495364482534	2.36514713159253	-1.80828512527555
H	4.46010055611411	2.47468080349658	-1.80430240692047
C	4.91001399943791	0.38660393629825	-0.13356155966516
H	5.50157784689865	1.13243884771022	-0.66651211005472
C	1.20748508515283	3.12537840381784	-2.58725808495374
H	0.61595955787774	3.82289379589918	-3.18426937863466
C	4.82075879245789	-1.52682004592447	1.35148906201237

H	5.34170744196164	-2.26320488019201	1.96777778090713
C	3.44455514361562	-1.54886275421874	1.25837298283962
H	2.84337332929519	-2.28995882004031	1.78917012939419
C	5.55445584971769	-0.55174169318832	0.65057553730897
H	6.64426942737725	-0.53506688886121	0.72600850031932
C	2.60998624223595	3.23817184909229	-2.55774691649634
H	3.10067892778343	4.02564788468339	-3.13465958322540
N	-1.34523654486856	-0.75086137367127	-1.13962109539762
C	-1.47134865877545	0.74340334705169	0.73249984126561
C	-0.74075836011201	0.04017176351059	-0.26538379306482
C	-3.52336884617957	-0.27350656103897	-0.16029477252715
C	-0.79505005993895	1.58293055969098	1.65194046409398
C	-2.88302747341056	0.59980616335036	0.79573467653353
C	-2.73227915223051	-0.94688507656330	-1.12359879717118
C	-3.58265038759895	1.31291776125551	1.78811905358616
H	-4.66596179526961	1.22657098121501	1.86789260445100
C	-4.91716215676301	-0.48988195246834	-0.17627888297352
H	-5.54804396401529	0.01578974973073	0.55446471592776
C	-1.50703436251860	2.26770095783316	2.61046865163488
H	-0.98825941749485	2.91465805635577	3.32052541617870
C	-4.70227373003112	-1.99532469890343	-2.04484367112430
H	-5.15902215049971	-2.66542178103179	-2.77617681733605
C	-3.33374600218174	-1.80746104932026	-2.06063721634590
H	-2.73685560871698	-2.33267194557836	-2.80300316310003
C	-5.49959122606883	-1.33377742128296	-1.09971218154466
H	-6.58083658307464	-1.48597528643887	-1.09226188608400
C	-2.90598434327654	2.12936458832432	2.67434155298021
H	-3.46755254237701	2.67368446918888	3.43721714192905
H	0.29008201304678	1.68082746611414	1.60083666641532
H	-0.50531603858451	2.04472526672541	-1.87777614888436
C	-0.56889094495051	-1.45413639360428	-2.16232052856031
H	-0.92390268899065	-1.15767564344736	-3.15701989378569
H	0.48808438241683	-1.19780217681206	-2.06791292561979

H -0.68514509207426 -2.53698878857143 -2.02835081292509

[biphe-Me]⁺ (4), S_{0,eq} in methanol

N	1.39397749341305	-0.68404127674651	0.39747172766182
C	1.35358304892259	1.23931718634984	-1.08056197679048
C	0.74871979603823	0.17958918084547	-0.32059981924295
C	3.50208858750505	0.38241584204978	-0.24565564577488
C	0.58954563794740	2.14724107277472	-1.84549205060421
C	2.76885327191817	1.34352810329738	-1.04217480641868
C	2.76323149187881	-0.61239113103188	0.45151336884030
C	3.38176204600068	2.37645435783672	-1.78291781648164
H	4.46716537848262	2.48526263953710	-1.77525487506247
C	4.90810363497361	0.37970069070128	-0.12459400351237
H	5.50184141182242	1.13236930048900	-0.64583969161066
C	1.21688688271152	3.14673586722211	-2.56001283415552
H	0.62738722761034	3.85097336102118	-3.15146006045692
C	4.81312109968833	-1.55163891184558	1.33594188518605
H	5.33107784049889	-2.29640093373901	1.94511219953397
C	3.43703601847376	-1.57163411130962	1.23730835224640
H	2.83581492523762	-2.32041764599274	1.75768172599213
C	5.54988219465089	-0.56820929071381	0.65034273425821
H	6.63964244015667	-0.55240824614498	0.73012176511410
C	2.61921954469141	3.25823269771423	-2.52491720817636
H	3.11237992986093	4.05174280977676	-3.09181124875681
N	-1.34720462277492	-0.75215871030068	-1.14566006546542
C	-1.47182025411239	0.75385926119525	0.71714473266831
C	-0.74291610203780	0.04411143269736	-0.27761623691492
C	-3.52211706217955	-0.28154006939948	-0.15665891728224
C	-0.79620971822783	1.60695774412377	1.62422775929158
C	-2.88217450704783	0.60473298106210	0.78713899708611
C	-2.73262660509278	-0.95695392191226	-1.11943052772825
C	-3.58204055110435	1.32479432968503	1.77448349374095
H	-4.66476874165234	1.23425980817622	1.85931144902788

C	-4.91447771049515	-0.50738595944425	-0.16127277195387
H	-5.54482639926447	-0.00003044662006	0.56908281339238
C	-1.50825402233204	2.29909676156648	2.57751255257623
H	-0.98986247466619	2.95768316672694	3.27740393335746
C	-4.69982339661468	-2.02775407414902	-2.01824976044404
H	-5.15612727138366	-2.70801313539361	-2.74072215124010
C	-3.33293996038993	-1.83017922936377	-2.04515356234585
H	-2.73677148408613	-2.35770599246536	-2.78668910692123
C	-5.49602128280401	-1.36355954485928	-1.07393247441139
H	-6.57631651245140	-1.52334085839630	-1.05836978160954
C	-2.90610479543074	2.15430731243528	2.64880992110026
H	-3.46761438963138	2.70454277759609	3.40771703543673
H	0.28811560639362	1.71333233306635	1.56827070507043
H	-0.49961226993350	2.05960382251313	-1.86955671401765
C	-0.57488017249978	-1.44547944192958	-2.17836052615656
H	-0.95404427143058	-1.15946930040488	-3.16705101809766
H	0.47806193969363	-1.16569845526196	-2.10736327260747
H	-0.66654287092678	-2.52993415303497	-2.03831822734116

[biphe-Me]⁺ (**4**), S_{0,eq} in dimethyl sulfoxide

N	1.40205556845173	-0.67034094253489	0.42697423083659
C	1.34897209495626	1.21776610154233	-1.09502785341263
C	0.75098382288065	0.17100327243524	-0.31154531441773
C	3.50318029849466	0.39258881490413	-0.24313303582908
C	0.57872595157508	2.10389317323352	-1.87883828338284
C	2.76340017743129	1.33243513902057	-1.05863724549586
C	2.77058501444026	-0.59047946848927	0.47722025728151
C	3.36937905081522	2.35467352075838	-1.81948611356701
H	4.45393238842025	2.47136028187449	-1.81237057232590
C	4.90933135473103	0.39932049854549	-0.12510643548488
H	5.49757358901453	1.14287141446146	-0.66520232252286
C	1.19936414531294	3.09302251121002	-2.61338161857254
H	0.60536150922984	3.78053497666010	-3.21957390613956

C	4.82657295971135	-1.49941375214381	1.37866608653773
H	5.34952362691808	-2.22767099307581	2.00311142863011
C	3.45041623201742	-1.52860584037776	1.28327492240112
H	2.85280192329058	-2.26810690933151	1.82067463513457
C	5.55712441596963	-0.52805713638860	0.66947008731433
H	6.64684551884964	-0.50556399207323	0.74633387111669
C	2.60082397638978	3.21571869706608	-2.57944216943739
H	3.08836406182608	4.00133863424648	-3.16172643517748
N	-1.34763694144281	-0.74825394825438	-1.14550465352406
C	-1.46579099322368	0.73058630872423	0.73933189143509
C	-0.74022888429718	0.03127205842068	-0.26508698549310
C	-3.52189988829916	-0.27196173444681	-0.15810666520043
C	-0.78529194093544	1.56350109900409	1.66126784445263
C	-2.87720228677559	0.59018876338139	0.80457359468287
C	-2.73496041938840	-0.93730784350842	-1.13019669053245
C	-3.57327978663820	1.29724804456451	1.80388444502811
H	-4.65669989113768	1.21290834517798	1.88545743611647
C	-4.91649339197692	-0.48287933500501	-0.17333341213860
H	-5.54458962673859	0.01625785995319	0.56444797349476
C	-1.49371982489804	2.24300606762301	2.62623999025132
H	-0.97188460388573	2.88560642659964	3.33811675645453
C	-4.70972323676459	-1.96587021284571	-2.06119409975839
H	-5.17017033032986	-2.62444591485637	-2.80071307310125
C	-3.34059438140095	-1.78354620844363	-2.07732954386888
H	-2.74662129971961	-2.30055416713761	-2.82783523724670
C	-5.50293008927407	-1.31356444714024	-1.10616396483360
H	-6.58481639724489	-1.46182761627647	-1.09872145754311
C	-2.89254979533545	2.10603065773577	2.69377933918226
H	-3.45106167558974	2.64618368067048	3.46188429212950
H	0.29969179429254	1.66281799311103	1.60742316075395
H	-0.50962271870899	2.00645524739593	-1.90214447609725
C	-0.57618265425045	-1.44322883969336	-2.17715964023643
H	-0.92408358707893	-1.12320968829951	-3.16701854113319

H	0.48387233875571	-1.20304011689720	-2.07411364212862
H	-0.70944716843954	-2.52616048110069	-2.06313885463230

[biphe-Me]⁺ (4), S_{0,eq} in water

N	1.38487064390886	-0.70986513416273	0.35678380878016
C	1.35905592466775	1.26660827876253	-1.05112345139487
C	0.74627954131469	0.18641197294958	-0.32794195602303
C	3.50083651137226	0.36376129865579	-0.25059327390741
C	0.60195165924570	2.20840386304009	-1.78140522466821
C	2.77511023186111	1.35605280612679	-1.01436620643211
C	2.75541673522057	-0.64857660155919	0.41274890675294
C	3.39649089136030	2.40523997333273	-1.72443572400507
H	4.48281323002270	2.50087742633533	-1.71878401817767
C	4.90683918578032	0.34914536468657	-0.13004878483621
H	5.50420627244966	1.11629879087151	-0.62472486682521
C	1.23715251075436	3.22413292785563	-2.46522121464446
H	0.65282797921047	3.95394215095263	-3.02934215295036
C	4.80059248664425	-1.62929056731204	1.26365675992315
H	5.31336820733034	-2.39720764179777	1.84712826819864
C	3.42444663918941	-1.63750959672584	1.16476140429819
H	2.82139993645118	-2.40055956785225	1.66061877435303
C	5.54347600446223	-0.62777898117069	0.61205163140726
H	6.63283335765251	-0.62066346762124	0.69255466729028
C	2.64077420127891	3.31868291243638	-2.43415279558083
H	3.14004714206874	4.12408662139949	-2.97758730363147
N	-1.34504267655357	-0.76002197599492	-1.14291302306078
C	-1.48147380526726	0.78812379174906	0.68393044286446
C	-0.74594390951235	0.05942257479398	-0.29223884495562
C	-3.52174729820038	-0.29366314213124	-0.15652874188729
C	-0.81512758354303	1.67301216851918	1.56709849648331
C	-2.89038329677825	0.62850879729886	0.75774394899365
C	-2.72725288186638	-0.98589866538771	-1.10234669465999
C	-3.59818145840298	1.37080498506999	1.72261315143862

H	-4.67987589031261	1.27216586481714	1.80818939220883
C	-4.91056731629559	-0.53954335636924	-0.14690887905966
H	-5.54410760473787	-0.01810176487497	0.57026196819397
C	-1.53460347364719	2.38701892404814	2.49833008123625
H	-1.02309420428703	3.07060006850017	3.17836189928884
C	-4.68098972969242	-2.11751043714427	-1.95341338742330
H	-5.12969203409672	-2.82979244320022	-2.64862482041830
C	-3.31765773724597	-1.89938870890103	-1.99470059633795
H	-2.71589035244722	-2.44412922807580	-2.71880741189252
C	-5.48317104900322	-1.43348871066807	-1.02837779972027
H	-6.56041206895692	-1.60882274599249	-1.00231689852031
C	-2.93121825119587	2.23218792398025	2.57245118224124
H	-3.49837498451076	2.79968778954967	3.31361279498315
H	0.26784010119464	1.78877617211787	1.50864159495871
H	-0.48795778618183	2.13580538940792	-1.80085036155905
C	-0.57140237718416	-1.45091831033846	-2.17718110405831
H	-1.00170715927626	-1.22356514862013	-3.15918215765623
H	0.46401350699877	-1.10627542092264	-2.15979034578053
H	-0.59536797124385	-2.53268722043439	-1.99673113382766

pBiphe (5), $S_{0,eq}$ in vacuum

N	1.34633039888446	0.03424427681131	-1.39783241965039
C	1.44199078301986	0.03880446814936	1.01611343991712
C	0.74116253077270	0.01933645481384	-0.24510912787526
C	3.52422578931314	0.09377813159908	-0.28957550349980
C	0.73622705921968	0.02029448445757	2.25110564778107
C	2.86089852858683	0.07714068973494	0.99470312183451
C	2.70446577335009	0.07035557842047	-1.45093208530352
C	3.56021497256317	0.09714623952920	2.21740782628740
H	4.64989610463856	0.12658984907572	2.22462229369317
C	4.92465020868766	0.13134574000927	-0.45354503923198
H	5.57645630880389	0.14999498328281	0.42120744612041
C	1.47308447019091	0.04154057311956	3.43175715390889

H	0.96788827532927	0.02882892613209	4.39732246314200
C	4.67763643587498	0.12154665246678	-2.86226166511311
H	5.13561148976165	0.13254299861096	-3.85399454832453
C	3.30658170944513	0.08487047629620	-2.73123121339309
H	2.63799346548387	0.06585199380105	-3.59355221232234
C	5.49111416057448	0.14496560409511	-1.71343443318993
H	6.57814023471257	0.17410535294332	-1.81769163743918
C	2.87120746320897	0.07963126837495	3.41333705200421
H	3.41954847726536	0.09547212906875	4.35789635795566
N	-1.34645043089505	-0.03435369329624	-1.39772698794851
C	-1.44192272064364	-0.03887925673647	1.01622645271370
C	-0.74119273370737	-0.01942932991124	-0.24505107889364
C	-3.52425954534297	-0.09387053942890	-0.28929952346764
C	-0.73606279897918	-0.02035209339121	2.25116335511126
C	-2.86083212068419	-0.07721552868556	0.99492712439763
C	-2.70458995144862	-0.07046510654081	-1.45072032323162
C	-3.56005339894894	-0.09720427531602	2.21768655500368
H	-4.64973397019901	-0.12664795389459	2.22498654892397
C	-4.92469676171494	-0.13143908377039	-0.45315940380536
H	-5.57643507408082	-0.15007501096967	0.42164388470402
C	-1.47282821344002	-0.04158183258364	3.43187257954631
H	-0.96755746385786	-0.02885689639350	4.39739866397815
C	-4.67787080977981	-0.12167473696969	-2.86189532210493
H	-5.13592248742947	-0.13268480942462	-3.85359266109266
C	-3.30680575045698	-0.08499788717085	-2.73097218221299
H	-2.63828554888569	-0.06599226183137	-3.59334619299558
C	-5.49125897156191	-0.14507640921517	-1.71300452353075
H	-6.57829327642283	-0.17421645976316	-1.81717589584623
C	-2.87095268580140	-0.07967285174930	3.41356183305006
H	-3.41921992540655	-0.09550085374993	4.35816418039986

pBiphe (**5**), S_{0,eq} in chloroform

N	1.34698867466540	0.03271043991109	-1.39764727905135
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C	1.44184033901899	0.04173174216878	1.01634018229345
C	0.74120114746871	0.01908652427384	-0.24326449290966
C	3.52467416537097	0.09378195683089	-0.29056733845452
C	0.73616346852488	0.02544829829962	2.25208917143541
C	2.86112453030487	0.08341419093493	0.99430545841164
C	2.70681944365584	0.06679671125990	-1.45343275754953
C	3.56262799713554	0.11320052682188	2.21602884434176
H	4.65250466080210	0.14587265711179	2.22266366626134
C	4.92619427338721	0.12797839756969	-0.45108938045430
H	5.57519480910841	0.14843809922881	0.42576870702616
C	1.47337407925433	0.05986155129879	3.43278178715802
H	0.97023289087415	0.05494623564745	4.39969801538350
C	4.68276249596806	0.10833363564620	-2.86176082504893
H	5.14231170731705	0.11397236732764	-3.85311940048396
C	3.31053863528359	0.07507790629567	-2.73332042618589
H	2.65012011610155	0.05374107653737	-3.60279808336850
C	5.49434510416276	0.13481026666473	-1.71108979468826
H	6.58189925703712	0.16070347305913	-1.81376987814339
C	2.87216565296894	0.10318608222810	3.41194201833949
H	3.42041697327144	0.12904105251270	4.35654815537408
N	-1.34710937877240	-0.03281974483020	-1.39754081743898
C	-1.44177259640698	-0.04180717251308	1.01645382699341
C	-0.74123157226364	-0.01918004931371	-0.24320582434327
C	-3.52470845862217	-0.09387518970724	-0.29029069683540
C	-0.73599926009513	-0.02550619295981	2.25214745415920
C	-2.86105859105318	-0.08348966113542	0.99453023207431
C	-2.70694430696076	-0.06690624672386	-1.45322009940612
C	-3.56246666046917	-0.11325834355311	2.21630885030419
H	-4.65234282252569	-0.14592982757040	2.22302981614992
C	-4.92624102271030	-0.12807328454815	-0.45070387188383
H	-5.57517414516866	-0.14852089099370	0.42620429454873
C	-1.47311763274311	-0.05990243263462	3.43289827307910
H	-0.96990135530421	-0.05497352206197	4.39977550936917

C	-4.68299626348730	-0.10846107603945	-2.86139463472741
H	-5.14262237514961	-0.11411282110937	-3.85271750739605
C	-3.31076249792606	-0.07520431925881	-2.73306094462105
H	-2.65041080904594	-0.05387937874429	-3.60258962905472
C	-5.49448948921726	-0.13492184888877	-1.71066021993806
H	-6.58205160231793	-0.16081588360695	-1.81325561453358
C	-2.87191087624792	-0.10322698711006	3.41216801880591
H	-3.42008870519452	-0.12906831832604	4.35681723500802

pBiphe (**5**), S_{0,eq} in methanol

N	1.34782206567851	0.03038661573929	-1.39956025493099
C	1.44134602881764	0.04315739437042	1.01472938651208
C	0.74117384325191	0.01851828408648	-0.24438277993792
C	3.52487047876274	0.09372749322464	-0.29091122762864
C	0.73578970859872	0.02802616331906	2.25056396276992
C	2.86064911032228	0.08665823748397	0.99328903668937
C	2.70864141816489	0.06379672453328	-1.45454960917768
C	3.56238348579423	0.12143989403513	2.21463114396375
H	4.65238632977351	0.15581036668373	2.22227748681557
C	4.92675719970485	0.12716869387957	-0.44855043227595
H	5.57432451118938	0.14965241745256	0.42947034742375
C	1.47239651028287	0.06878039840503	3.43136572208417
H	0.96993901260948	0.06723217222304	4.39883289385855
C	4.68736573642229	0.10095271434887	-2.85949737902819
H	5.14849119405021	0.10365245919542	-3.85034584614445
C	3.31475793475206	0.06849129263267	-2.73329703021906
H	2.65930039395983	0.04504113744939	-3.60682910827813
C	5.49709984564027	0.13031196222958	-1.70761607257588
H	6.58498922700250	0.15544434895432	-1.80855206114676
C	2.87122783723828	0.11491322252208	3.41022842202806
H	3.41917945834629	0.14565431253395	4.35500730681742
N	-1.34794305786642	-0.03049596489947	-1.39945344780160
C	-1.44127850255446	-0.04323243955656	1.01484319079888

C	-0.74120444337676	-0.01861137740885	-0.24432395219287
C	-3.52490495001405	-0.09382035024110	-0.29063441265903
C	-0.73562564911270	-0.02808369090530	2.25062235673821
C	-2.86058339557011	-0.08673336339454	0.99351402807247
C	-2.70876644432690	-0.06390628305134	-1.45433663692663
C	-3.56222234311217	-0.12149784921318	2.21491150891917
H	-4.65222458739594	-0.15586808722024	2.22264428480325
C	-4.92680390079823	-0.12726290204772	-0.44816495095026
H	-5.57430386726672	-0.14973403179239	0.42990568331313
C	-1.47214015126563	-0.06882134035600	3.43148240384117
H	-0.96960750079870	-0.06725987875906	4.39891068981344
C	-4.68759913355462	-0.10108046322692	-2.85913099861472
H	-5.14880134535207	-0.10379357947619	-3.84994372195878
C	-3.31498163599975	-0.06861808164000	-2.73303719441747
H	-2.65959098892051	-0.04518023547920	-3.60661976560267
C	-5.49724391413443	-0.13042325352581	-1.70718651333144
H	-6.58514109239959	-0.15555629786810	-1.80803797262583
C	-2.87097318426724	-0.11495445091279	3.41045474578294
H	-3.41885124227576	-0.14568238432771	4.35527676737969

pBiphe (**5**), $S_{0,eq}$ in dimethyl sulfoxide

N	1.34732898742450	0.03067889019812	-1.39877827980886
C	1.44158543929062	0.04305633278183	1.01558786619336
C	0.74133723381106	0.01858807342870	-0.24360799587432
C	3.52460671507997	0.09371922763243	-0.29078483869400
C	0.73585486022629	0.02787242465568	2.25129301577015
C	2.86083273279388	0.08642550079172	0.99371572262283
C	2.70783287307425	0.06409620350048	-1.45441072045188
C	3.56272043873802	0.12088111965481	2.21495558103279
H	4.65266962673678	0.15508541329266	2.22203939904254
C	4.92633533969629	0.12711636844932	-0.44923426795894
H	5.57400948847359	0.14937283856621	0.42863418007144
C	1.47265631657565	0.06830360286965	3.43196952967412

H	0.97007085256220	0.06662486866850	4.39929983078444
C	4.68569063173231	0.10146486616603	-2.86035083014206
H	5.14653966405741	0.10437000900201	-3.85118032412178
C	3.31313819534400	0.06904982823645	-2.73366613351233
H	2.65623130975537	0.04580923978168	-3.60604067989702
C	5.49585246664361	0.13050836706597	-1.70871206283540
H	6.58355259082991	0.15559794965282	-1.81022868811870
C	2.87154061395256	0.11420800095942	3.41057966445044
H	3.41946796921283	0.14466348754483	4.35522431944565
N	-1.34744992353275	-0.03078800626000	-1.39867151685485
C	-1.44151783832287	-0.04313131049635	1.01570171046736
C	-0.74136777798460	-0.01868100938821	-0.24354915231488
C	-3.52464116166670	-0.09381214300461	-0.29050805512582
C	-0.73569074621451	-0.02792988051660	2.25135143910774
C	-2.86076697387392	-0.08650065263914	0.99394072743845
C	-2.70795789665399	-0.06420562998194	-1.45419781307215
C	-3.56255926566919	-0.12093912854107	2.21523595553269
H	-4.65250789484298	-0.15514324641141	2.22240618595436
C	-4.92638206289335	-0.12721079116867	-0.44884883609019
H	-5.57398889461492	-0.14945483015414	0.42906943607906
C	-1.47239990840391	-0.06834444556671	3.43208626424461
H	-0.96973933419838	-0.06665239292107	4.39937769839695
C	-4.68592409934108	-0.10159263423689	-2.85998455725109
H	-5.14684990025844	-0.10451113273816	-3.85077830172871
C	-3.31336193739804	-0.06917649236238	-2.73340641154373
H	-2.65652185139467	-0.04594805981115	-3.60583154341284
C	-5.49599661055914	-0.13061984221391	-1.70828259597010
H	-6.58370459096128	-0.15571024003165	-1.80971470899343
C	-2.87128593221989	-0.11424921276897	3.41080600625291
H	-3.41913974500650	-0.14469153168631	4.35549378121124

pBiphe (5), $S_{0,eq}$ in water

N	1.35011863486922	0.02921306823600	-1.40356763199556
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C	1.44041410059974	0.04367644211785	1.01081158643236
C	0.74112329615220	0.01826686299409	-0.24865535574841
C	3.52554394578308	0.09383003975744	-0.29122177066228
C	0.73537924997115	0.02882706327762	2.24670515597861
C	2.85954956666198	0.08780148633802	0.99147234151349
C	2.71185262420489	0.06253158423932	-1.45582343237839
C	3.56084035898641	0.12409731330914	2.21291692576289
H	4.65056212698912	0.15898046917719	2.21976677084938
C	4.92785446288575	0.12741376546920	-0.44434909652837
H	5.57144053077515	0.15094836849515	0.43619660501679
C	1.47081019245763	0.07132246333584	3.42804237175585
H	0.96664911771436	0.07039017201499	4.39432815318995
C	4.69510022224775	0.09844354995041	-2.85498350583516
H	5.15819615478850	0.10007435175196	-3.84443366457946
C	3.32217853173471	0.06591244432369	-2.73235866347283
H	2.67180601475099	0.04145860046305	-3.60902186871262
C	5.50212687063039	0.12926846696840	-1.70139111719478
H	6.58983376196623	0.15446523050463	-1.79940701509319
C	2.86948771126540	0.11844891879202	3.40826800622428
H	3.41654574551243	0.15054349638476	4.35300809497503
N	-1.35023987896061	-0.02932287978892	-1.40346078757084
C	-1.44034683409496	-0.04375165040141	1.01092528515131
C	-0.74115421617332	-0.01836029336752	-0.24859660885649
C	-3.52557834505290	-0.09392281974464	-0.29094500859164
C	-0.73521547264229	-0.02888471977918	2.24676350452856
C	-2.85948392896712	-0.08787667009560	0.99169717531327
C	-2.71197771034041	-0.06264146231195	-1.45561035933507
C	-3.56067934510079	-0.12415545443439	2.21319709840453
H	-4.65040057380629	-0.15903859800813	2.22013332783133
C	-4.92790072401043	-0.12750733609212	-0.44396352556116
H	-5.57141912105400	-0.15102876634776	0.43663182247990
C	-1.47055410483326	-0.07136347540815	3.42815892016031
H	-0.96631803911206	-0.07041786352318	4.39440573594461

C	-4.69533336376289	-0.09857126431952	-2.85461654332247
H	-5.15850603256708	-0.10021549194683	-3.84403077887509
C	-3.32240222893933	-0.06603962809562	-2.73209836316550
H	-2.67209692856480	-0.04159842322510	-3.60881174392562
C	-5.50227047029486	-0.12937913247170	-1.70096110523360
H	-6.58998495793859	-0.15457610435850	-1.79889238772639
C	-2.86923322109900	-0.11849030267188	3.40849414758355
H	-3.41621772363214	-0.15057182150864	4.35327730526896

pBiphe (**5**), $T_{1,eq}$ in vacuum

N	1.34002165131729	0.03552526027873	-1.42766600931970
C	1.41777025568843	0.03768177813282	1.02116244756674
C	0.71053013498913	0.01883747096841	-0.21964286957966
C	3.50448741754580	0.09313241810557	-0.29085411341785
C	0.71749387778796	0.01908612527413	2.26362024591503
C	2.84445402550560	0.07563907661401	1.00113126013909
C	2.66935941447643	0.07086697643130	-1.46354087060969
C	3.53887486431576	0.09418728295917	2.21126968987394
H	4.62889511783725	0.12319883625640	2.21699414109469
C	4.89731936711153	0.13016998572559	-0.45881489147357
H	5.55094405928851	0.14759374186136	0.41486690602611
C	1.47619285440268	0.03936997386219	3.46513258872758
H	0.96972712646182	0.02599016180844	4.42958053695967
C	4.65801122756488	0.12367890235433	-2.87640589211537
H	5.12071181977019	0.13593329634999	-3.86595541995257
C	3.29118938387295	0.08733610721237	-2.75121439800053
H	2.62393293290072	0.06954990615017	-3.61452890689640
C	5.46984254626904	0.14533131520169	-1.72166379274223
H	6.55715945541151	0.17424394701800	-1.82161036864741
C	2.85192913170776	0.07600030755624	3.43481318611548
H	3.41632010983037	0.09110566343983	4.36965382622233
N	-1.34014414274584	-0.03563353001480	-1.42756105614055
C	-1.41770193704294	-0.03775610495570	1.02127347896138

C	-0.71055845910975	-0.01892899756761	-0.21958721552382
C	-3.50452129102342	-0.09322517623667	-0.29057961134191
C	-0.71732881126180	-0.01914317877097	2.26367646424157
C	-2.84438724982621	-0.07571387269214	1.00135402414142
C	-2.66948467443172	-0.07097583926409	-1.46333175881504
C	-3.53871381456213	-0.09424541310818	2.21154678720131
H	-4.62873360657072	-0.12325698983649	2.21735660869591
C	-4.89736633453318	-0.13026505004524	-0.45843139303575
H	-5.55092297419771	-0.14767676355796	0.41530154403593
C	-1.47593413781270	-0.03941040774642	3.46524820300330
H	-0.96939317120815	-0.02601717416957	4.42965644744157
C	-4.65824661827107	-0.12380722918936	-2.87604107572666
H	-5.12102431392847	-0.13607519429508	-3.86555437269765
C	-3.29141503922222	-0.08746269665245	-2.75095657814907
H	-2.62422589299626	-0.06968831804720	-3.61432333716853
C	-5.46998793782872	-0.14544375322070	-1.72123542898481
H	-6.55731263575029	-0.17435771416429	-1.82109684993850
C	-2.85167278518910	-0.07604134560856	3.43503650064630
H	-3.41599094654326	-0.09113378441729	4.36992132326792

pBiphe (5), S_{1,eq} in vacuum

N	1.31783443252294	0.03713429475398	-1.39656255922346
C	1.44681109613179	0.00924371146092	1.04992669592796
C	0.74349468562093	0.00652607024181	-0.19684785152947
C	3.50338728445299	0.08118140928309	-0.29927808361146
C	0.74449149446507	-0.02530532880542	2.28890641388765
C	2.86643188852703	0.04758725160358	1.00699942179077
C	2.66704309672843	0.07376499478670	-1.46025970904146
C	3.57118738823352	0.05091308514886	2.21986123487898
H	4.66110000956080	0.07993544418229	2.22134645159760
C	4.89860879218043	0.12051998245274	-0.47684723819583
H	5.55350278137918	0.12683659562305	0.39612632509227
C	1.49879162455743	-0.02018989665877	3.46942461635915

H	1.00141321503849	-0.04570543451309	4.43935779071640
C	4.64208334276877	0.14429562138113	-2.88017356200353
H	5.09137141046909	0.16888719165757	-3.87596377572932
C	3.27187515367594	0.10617942939144	-2.74319596840831
H	2.60456166841402	0.09947615985969	-3.60674909125578
C	5.46502490440198	0.15162370895940	-1.73901485311551
H	6.55134342637443	0.18184856968524	-1.84732428532142
C	2.88944051979703	0.01737024915749	3.43059919373165
H	3.45209664260704	0.02049488829694	4.36685508598296
N	-1.39254548543073	-0.03603394608442	-1.27412806078038
C	-1.42751807319621	-0.06721006096754	1.05709914504888
C	-0.67664471332894	-0.03143189524419	-0.16723394963176
C	-3.51574003001019	-0.10524014723188	-0.30405539021438
C	-0.71546070310196	-0.06430129975042	2.29029610673440
C	-2.85086010178126	-0.10439105407217	0.99722122432348
C	-2.69576185679856	-0.06803534564744	-1.49014270033773
C	-3.55384950974558	-0.13887366945190	2.20650676661458
H	-4.64354037650146	-0.16789562778246	2.20762893219537
C	-4.90223622126033	-0.13977964823689	-0.49364548531175
H	-5.54866191031955	-0.16832628765883	0.38543142730275
C	-1.48163919962442	-0.10014996570662	3.46518862796499
H	-0.98545746417322	-0.09972902638924	4.43581194865599
C	-4.65945317902252	-0.10234049635498	-2.89259029501589
H	-5.10835795851220	-0.10147004421546	-3.88860351432056
C	-3.28430075287386	-0.06714412397967	-2.77497538145411
H	-2.63057041025338	-0.03844807582925	-3.64663439447913
C	-5.47907332736003	-0.13888296679009	-1.75585693140538
H	-6.56476105400903	-0.16651500685696	-1.85977490401776
C	-2.86912586078608	-0.13651060528130	3.41967451742029
H	-3.43482791681780	-0.16383240041696	4.35366384617828

[pBiphe-H]⁺ (**6**), S_{0,eq} in vacuum

C	-6.14199581097694	-3.88483236850987	-0.06145469667359
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C	-4.76821095209425	-3.75016309890246	-0.06289867016679
C	-4.20555267791102	-2.46430617789390	-0.06178662839215
C	-5.01003252064717	-1.29771373763685	-0.05919902871318
C	-6.40745124866679	-1.47803510871893	-0.05778884071020
C	-6.96255655959122	-2.74367911375289	-0.05889766861633
C	-4.36376697475712	0.00188058955172	-0.05816649017932
C	-2.93917126761885	0.06183069039776	-0.05982393225171
C	-2.21255730359141	-1.15064718339887	-0.06238998131179
C	-2.22945587284998	1.30027952311082	-0.05898581952628
C	-2.98759256104033	2.46597558903361	-0.05643017799078
C	-4.38652212781119	2.41625588575704	-0.05477357300564
C	-5.07230939107562	1.21318895947981	-0.05561139050787
H	-6.59027389459514	-4.88021109439426	-0.06230905870612
H	-4.11594670722527	-4.62634018459312	-0.06489439932854
H	-7.06605249617896	-0.60960780664874	-0.05580150487521
H	-8.04814876138918	-2.85773461419479	-0.05777426315145
H	-2.50221765791224	3.44159671531019	-0.05567421021188
H	-4.94906794463038	3.35237763053817	-0.05277772059323
H	-6.16173271635451	1.21894006012438	-0.05426976944412
C	-0.75712484405468	-1.17622133053804	-0.06421911072794
C	-0.05469161216436	0.06551203093586	-0.06339111805255
C	1.15593003257781	-2.44961371184581	-0.06837472133863
C	1.36128468534235	0.01142454361815	-0.06524287467726
C	-0.75823041517846	1.30084068157637	-0.06081842677985
C	1.73512996322469	-3.74141139721599	-0.07089203349779
C	1.99223098804243	-1.28811859000354	-0.06783353613184
C	2.07376457023810	1.22911850658798	-0.06446381813243
C	-0.00781854847497	2.47154252803442	-0.06016233370962
C	3.10264728508840	-3.88818111178504	-0.07283847059247
H	1.06337918740515	-4.60122556026286	-0.07122584951676
C	3.38864522455583	-1.47697175834750	-0.06987817039487
C	1.39398792666843	2.43095172303199	-0.06197211070405
H	3.16368789417577	1.23049061663799	-0.06582394469070

H	-0.49778598078283	3.44538743738909	-0.05822576104493
C	3.93092585228969	-2.74731550504849	-0.07232406957205
H	3.54969616181269	-4.88423717495399	-0.07478471218360
H	4.05699855662358	-0.61554761049799	-0.06954776226282
H	1.95331585413593	3.36854552792490	-0.06139267098220
H	5.01621026933941	-2.86897171905744	-0.07388050149008
N	-2.84009416224145	-2.31446242470335	-0.06323325903669
N	-0.19678089161783	-2.35755617851326	-0.06654589652578
H	-2.20939255008803	-3.12503467762224	-0.06512102359889

[pBiphe-H]⁺ (6), S_{0,eq} in chloroform

C	-6.14499884441382	-3.88095331103489	-0.06320667043038
C	-4.77121521934421	-3.74893387075737	-0.06477039710298
C	-4.20984199257627	-2.46167903693972	-0.06282197105572
C	-5.01315213554028	-1.29498108301772	-0.05926087905780
C	-6.41156429956612	-1.47178245415770	-0.05773857308521
C	-6.96529243484633	-2.73826096979572	-0.05968189326385
C	-4.36394259190536	0.00170260097218	-0.05743931254850
C	-2.93976913168523	0.05801395992497	-0.05967879150107
C	-2.21561233035914	-1.15727054971051	-0.06287998112403
C	-2.23101925974527	1.29638496000848	-0.05844933613684
C	-2.98691319024322	2.46342871812417	-0.05405236200296
C	-4.38674424395765	2.41504777909200	-0.05167772671531
C	-5.07364741892300	1.21351015410707	-0.05348633401137
H	-6.59483235410201	-4.87606490036278	-0.06471481342052
H	-4.11248246175814	-4.62021366785782	-0.06750060375731
H	-7.06721286677881	-0.60073171732101	-0.05505049352004
H	-8.05138142034575	-2.85196994609171	-0.05848356362571
H	-2.50109059575598	3.43906574715751	-0.05221642661586
H	-4.94765196106480	3.35235703454314	-0.04832178732276
H	-6.16346033685758	1.21653147390686	-0.05163498370248
C	-0.75721370581253	-1.18272435891780	-0.06442780924395
C	-0.05529363151307	0.06102436342797	-0.06392247633825

C	1.16163072538821	-2.44907573965205	-0.06780918953533
C	1.36121160021188	0.01009965592423	-0.06610170435177
C	-0.75877490838542	1.29678528772188	-0.06162091686357
C	1.74253277977983	-3.73983297991641	-0.06933278408870
C	1.99535502289066	-1.28865096621635	-0.06778745078949
C	2.07501447313302	1.22663676029703	-0.06655036900780
C	-0.00885100097390	2.46841452326824	-0.06262354122244
C	3.11148118991274	-3.88415718203227	-0.07071174942003
H	1.07259894377272	-4.60194846808548	-0.06929150631718
C	3.39337216151892	-1.47269267939826	-0.06930272106800
C	1.39307395284622	2.42764277213809	-0.06505806975561
H	3.16530413308319	1.22592777373778	-0.06827701298788
H	-0.49907268108139	3.44227386305859	-0.06171876432717
C	3.93832409108282	-2.74234049010974	-0.07069110594942
H	3.55970314395915	-4.88024944665504	-0.07180488109516
H	4.05684058593635	-0.60703459854379	-0.06928410958524
H	1.95139132476602	3.36625542817579	-0.06574534411878
H	5.02423477011371	-2.86201577408703	-0.07176056502254
N	-2.84615173036865	-2.31607547324816	-0.06424022183768
N	-0.19296032358412	-2.36014969620548	-0.06636746103139
H	-2.23662582690730	-3.14331349547112	-0.06640334604189

[pBiphe-H]⁺ (6), S_{0,eq} in methanol

C	-6.14794847101300	-3.87806890120171	-0.07287869536625
C	-4.77420383617725	-3.74770699983620	-0.07717046209463
C	-4.21239581698066	-2.46072668357205	-0.06661186112625
C	-5.01429876713497	-1.29381518498989	-0.05121022166300
C	-6.41301607886094	-1.46830859808813	-0.04696687793044
C	-6.96728939020210	-2.73444659650456	-0.05779944320446
C	-4.36350140024449	0.00100556303100	-0.04137961136261
C	-2.93966096467055	0.05536784907350	-0.05324506846592
C	-2.21645867905918	-1.16072495329464	-0.06483199167509
C	-2.23115829524704	1.29343012127138	-0.04923696496611

C	-2.98538670463407	2.46103616648435	-0.02246084572111
C	-4.38533287904601	2.41363283311356	-0.00839702598984
C	-5.07293645058526	1.21296868105356	-0.01975220136797
H	-6.59900013500262	-4.87283184538436	-0.08136517789840
H	-4.11452251055714	-4.61829544174460	-0.08884956485302
H	-7.06771562305214	-0.59637345550296	-0.03581372027742
H	-8.05370577601197	-2.84731749486095	-0.05483228540817
H	-2.49922081039355	3.43661631021236	-0.01013294111974
H	-4.94539345696125	3.35139916204053	0.01188951801042
H	-6.16290597291040	1.21620319594396	-0.00960458494729
C	-0.75734645418991	-1.18645123049338	-0.06747965027799
C	-0.05592455518607	0.05795923782843	-0.07328452564308
C	1.16416721915758	-2.44928659255063	-0.07096178835048
C	1.36054591564938	0.00883144740483	-0.08492122312777
C	-0.75938437184103	1.29365004224392	-0.07125491720369
C	1.74736378654026	-3.73879117154472	-0.06554021822341
C	1.99616249059952	-1.28888701204677	-0.08053682907100
C	2.07428867832734	1.22499973757466	-0.10079992979080
C	-0.01040032134110	2.46572669509285	-0.09213017178237
C	3.11683137708229	-3.88113022726523	-0.06882923318190
H	1.07988584063827	-4.60309502284807	-0.05826516227658
C	3.39477674633931	-1.46980878447811	-0.08437536793873
C	1.39137298855841	2.42545547120256	-0.10657602364091
H	3.16474701733643	1.22481438669692	-0.11078343748377
H	-0.50089422336542	3.43957639009933	-0.09971046401409
C	3.94213322543176	-2.73841918065980	-0.07831183667203
H	3.56622448584991	-4.87698227445639	-0.06400609285435
H	4.05638843289839	-0.60247230899964	-0.09119365613251
H	1.94906685067064	3.36454143874856	-0.12244593786937
H	5.02847885259592	-2.85626495246551	-0.08066103846497
N	-2.84884600482251	-2.31787061157216	-0.07030582131407
N	-0.19144441719767	-2.36292255672458	-0.06736261883246
H	-2.24711519698709	-3.15083034303116	-0.07664589642634

[pBiphe-H]⁺ (6), S_{0,eq} in dimethyl sulfoxide

C	-6.14669669623826	-3.87852049731820	-0.07247973947023
C	-4.77298287361854	-3.74805235773511	-0.07691629041304
C	-4.21141792527649	-2.46084209277939	-0.06648895831618
C	-5.01379134444234	-1.29392494645918	-0.05113407989896
C	-6.41238432353233	-1.46873184426755	-0.04666414438268
C	-6.96626194329710	-2.73504853282841	-0.05734189008731
C	-4.36346810099343	0.00115685256152	-0.04159503139646
C	-2.93976886348333	0.05587261660254	-0.05337698830658
C	-2.21665951450778	-1.16033922607622	-0.06487350242754
C	-2.23123816438076	1.29386420451295	-0.04945373807382
C	-2.98564319608797	2.46134623435777	-0.02308232379572
C	-4.38560438483433	2.41372608120792	-0.00923175532355
C	-5.07313063594706	1.21298659074625	-0.02034415543901
H	-6.59754964272180	-4.87322164092902	-0.08088241876909
H	-4.11279297130079	-4.61811349603473	-0.08858886392272
H	-7.06695334236175	-0.59679199085220	-0.03541535367299
H	-8.05251572296533	-2.84814453720510	-0.05420036569823
H	-2.49917336213374	3.43670190745506	-0.01094200917274
H	-4.94573878855715	3.35129295750481	0.01066522839096
H	-6.16303076297885	1.21569810964053	-0.01038841041027
C	-0.75725722196583	-1.18586688692195	-0.06755785944621
C	-0.05577945491898	0.05869029022969	-0.07322599814046
C	1.16350583385122	-2.44901267945092	-0.07114149385807
C	1.36065267246669	0.00926267304676	-0.08471499357245
C	-0.75938165315021	1.29421963155118	-0.07113522329691
C	1.74586763797963	-3.73897476122317	-0.06587292161844
C	1.99599858465712	-1.28868212537357	-0.08058439721025
C	2.07448324713505	1.22532204779134	-0.10017451583132
C	-0.01027929532904	2.46623681057264	-0.09158177849127
C	3.11529996296522	-3.88178623157283	-0.06922891421763
H	1.07708409512066	-4.60218360153088	-0.05867562263876

C	3.39443395943799	-1.47033419507520	-0.08454062916766
C	1.39149480470042	2.42581262190579	-0.10574810937933
H	3.16487738406805	1.22470913938672	-0.10990502099905
H	-0.50113683311845	3.43982881021377	-0.09899885266253
C	3.94102450060796	-2.73933832976785	-0.07864625226926
H	3.56432965358453	-4.87765461061295	-0.06452288538806
H	4.05617996726806	-0.60317915708443	-0.09135056314850
H	1.94919397607266	3.36474358828261	-0.12119658792453
H	5.02717912442207	-2.85767374991346	-0.08108332658549
N	-2.84831007347323	-2.31741136054546	-0.07029050514051
N	-0.19168147688207	-2.36203526295262	-0.06749158956860
H	-2.24595049184036	-3.15022074805941	-0.07662903685856

[pBiphe-H]⁺ (6), S_{0,eq} in water

C	-6.15244535102626	-3.87490534654524	-0.05083560567910
C	-4.77860547016261	-3.74618032541706	-0.04993779368322
C	-4.21563674518497	-2.46004340026076	-0.05784820316275
C	-5.01571025849958	-1.29267604086994	-0.06714826156142
C	-6.41461869844396	-1.46476882803729	-0.06818426305568
C	-6.97044896736193	-2.73017442550096	-0.05995037748042
C	-4.36303617843102	0.00066340607533	-0.07444647463061
C	-2.93921173129673	0.05295022342737	-0.06659772524955
C	-2.21653306885173	-1.16359483439911	-0.06094379279296
C	-2.23092876137897	1.29072189339454	-0.06869528834741
C	-2.98395772673402	2.45911705824786	-0.08912346270039
C	-4.38386889465613	2.41327331990505	-0.09909087127442
C	-5.07190709807464	1.21291992059566	-0.08978683624298
H	-6.60453418340884	-4.86873120218046	-0.04432208132862
H	-4.11903201639927	-4.61647667239624	-0.04298163920536
H	-7.06702084154829	-0.59139121571148	-0.07481665160868
H	-8.05657750552637	-2.84166142967930	-0.06033722467410
H	-2.49595811981048	3.43351023922127	-0.09944714141909
H	-4.94300941128191	3.35116501738675	-0.11438099070802

H	-6.16165405141938	1.21541925349807	-0.09650607061213
C	-0.75751281373614	-1.19041239544204	-0.06210473133713
C	-0.05683036120178	0.05438380693968	-0.05442048154769
C	1.16628115207596	-2.45071887138493	-0.06661886092875
C	1.35944197800099	0.00700980064659	-0.04652403611185
C	-0.75973614628072	1.29022646343322	-0.05117050627703
C	1.75353351153212	-3.73818064836308	-0.07664444346100
C	1.99622610616886	-1.28955955706897	-0.05553303615350
C	2.07313755942640	1.22306073082261	-0.02973034106149
C	-0.01146274537534	2.46261384749287	-0.02968412578710
C	3.12334761746849	-3.87728313150498	-0.07615618700490
H	1.09071239159088	-4.60539141463674	-0.08500013591274
C	3.39531177467959	-1.46633247191828	-0.05460208069902
C	1.39022791263956	2.42338750911064	-0.01934394420570
H	3.16334240825903	1.22188412764452	-0.02288131327630
H	-0.50352163182837	3.43533689880659	-0.01855745337741
C	3.94633876808223	-2.73309651554156	-0.06498877739066
H	3.57434503818523	-4.87191020239301	-0.08443214402230
H	4.05323553834662	-0.59656093129030	-0.04646570214455
H	1.94733749217717	3.36229987764418	-0.00302002939060
H	5.03253423856341	-2.84821111749644	-0.06474066105900
N	-2.85147362205647	-2.31978529318510	-0.05735230585569
N	-0.19042686298568	-2.36717047654474	-0.06710898424946
H	-2.25434536123493	-3.15498882352474	-0.05514745032924

[pBiphe-Me]⁺ (7), S_{0,eq} in vacuum

N	1.39756934357335	-0.10787480590873	-1.37061956018641
C	1.46786692413136	0.15564415258247	1.02560322314153
C	0.77937795911549	0.08318356511449	-0.23198719006948
C	3.55932221230774	0.00366547974247	-0.25668205776310
C	0.75532021695885	0.18641162695842	2.24895465612882
C	2.88691033138688	0.16755870713459	1.00891338983909
C	2.74821218339156	-0.17559336140265	-1.41708828223322

C	3.57371054793398	0.30716392878041	2.23189759411115
H	4.66314717897362	0.33355474268028	2.24889551444942
C	4.95934227643756	-0.02133025429472	-0.41105090515036
H	5.61000429556507	0.12097176991400	0.45217928028307
C	1.47658148649857	0.32625560202575	3.43169074982039
H	0.96428866289616	0.37475811796971	4.39236842474995
C	4.72355037503260	-0.43270555282418	-2.79375120359955
H	5.19186553815412	-0.60573404282793	-3.76469471387615
C	3.35347365980758	-0.40277061186017	-2.67822159804313
H	2.69886973241176	-0.54656962479832	-3.53926975570506
C	5.52738761228036	-0.23456735581607	-1.65234058897910
H	6.61507684587399	-0.25392870096408	-1.74943734016180
C	2.87381133519328	0.40249983709713	3.41831408733989
H	3.41333463199854	0.51813700776910	4.36028243115880
N	-1.36302164735164	0.35625044763371	-1.39586070179764
C	-1.39992305452036	-0.01786379929549	0.97598596225174
C	-0.68838674985067	0.15524462853331	-0.24958677540272
C	-3.47625172784951	-0.21972898662049	-0.33204771149307
C	-0.69914842846957	0.02114683214468	2.22251467375381
C	-2.81530091187484	-0.16800266831937	0.95122210685695
C	-2.72816930923635	0.06609949109691	-1.49702799555069
C	-3.51323600285771	-0.27646502470516	2.16238816525515
H	-4.59732242750536	-0.37954415534900	2.16718863028421
C	-4.84353359271673	-0.53033386450796	-0.47300496254404
H	-5.43473431176360	-0.76625183530024	0.41114561086538
C	-1.44176644999543	-0.09440865179491	3.39373903951041
H	-0.94268301528761	-0.07391528216295	4.36161946481128
C	-4.69476258446779	-0.28164747112400	-2.86112675554346
H	-5.16097437333156	-0.32424180585753	-3.84737687063593
C	-3.35287022513467	0.03014321362932	-2.75917438050219
H	-2.78503668526921	0.20926644828756	-3.66942243405268
C	-5.44897919806625	-0.55855894202027	-1.71256153212560
H	-6.50827891827115	-0.80724845381981	-1.79801665530538

C	-2.82942034988258	-0.24126565493184	3.36375384517352
H	-3.37986128995331	-0.32669049761470	4.30295830344047
C	-0.74020636300036	0.97237347515234	-2.57334631128769
H	0.14085526323484	1.53771432593294	-2.26829912115713
H	-0.42770725875589	0.21891531981766	-3.30595830208022
H	-1.47610373774510	1.65568268412331	-3.01206144797919

[methylene-pBiphe]²⁺ (**8**), S_{0,eq} in vacuum

N	1.09265235174910	0.25986735576828	-1.23982733959293
C	1.42472098554716	0.05133601995843	1.15904055209091
C	0.66628642505579	0.09307993509177	0.00604582014942
C	3.33101191249736	0.38972657454451	-0.35568925055947
C	0.73793938819374	-0.14036989339930	2.40079112040419
C	2.82668213542559	0.20450980819352	0.99735489528916
C	2.44570762715915	0.41734133969429	-1.49125430473647
C	3.59139074873499	0.16064163087160	2.17801630824637
H	4.67601490154056	0.26847658783819	2.15809201543334
C	4.70489479686319	0.55088395216676	-0.62428933201868
H	5.41736140547504	0.53766135458692	0.20082441982305
C	1.55289842056703	-0.17337763988162	3.52273836244989
H	1.13410737412377	-0.31431714459052	4.52052569613307
C	4.28238421458206	0.74828206917326	-3.00161976476073
H	4.66417596166490	0.88729883447872	-4.01519856199566
C	2.92451205059729	0.59506803472870	-2.79579050836450
H	2.23682181748590	0.61308513966200	-3.64361979040638
C	5.17238278173506	0.72586437733251	-1.91297550836014
H	6.24314388097839	0.84792158414479	-2.08804612404117
C	2.95192285657762	-0.02407640966507	3.39606607204110
H	3.55735666511406	-0.05618783123417	4.30501304708402
N	-1.19254624125769	0.03669697821848	-1.23095585144744
C	-1.45941853002011	-0.23095528126140	1.17020231015922
C	-0.73238113158950	-0.04351744547681	0.01147387036228
C	-3.40667370551005	-0.26984441250323	-0.32962833572556

C	-0.73897426635169	-0.28506937913440	2.40648466951295
C	-2.86565950528570	-0.35283942479041	1.01936751691472
C	-2.55229745724042	-0.07167697353322	-1.47190703091196
C	-3.59824797593335	-0.54360761775834	2.20578542605979
H	-4.68331493599238	-0.64815814328234	2.19429505884318
C	-4.78772596077661	-0.37839281838933	-0.58755348612609
H	-5.47773348440777	-0.52906374782097	0.24297925097258
C	-1.52340101425009	-0.47505999499131	3.53457199856327
H	-1.07761150763924	-0.53168759705437	4.52900317112750
C	-4.42987521969540	-0.10414417327833	-2.96785754822343
H	-4.83910607271507	-0.04241851273083	-3.97837785614826
C	-3.06652308940723	0.00906556930323	-2.77256532128767
H	-2.40198337128168	0.15963965921287	-3.62566006255491
C	-5.29021883368853	-0.29808533677199	-1.87244679348722
H	-6.36565256759577	-0.38600583015350	-2.03914431542796
C	-2.92574570919163	-0.60009702537550	3.41873496994734
H	-3.50643120814815	-0.74861176423384	4.33225282221348
C	-0.06246113366114	0.23971388424833	-2.15649564941931
H	-0.15794921251398	1.19703087672739	-2.69389502927056
H	0.01596343248542	-0.59302716863375	-2.87396160895438

[ethylene-pBiphe]²⁺ (**9**), S_{0,eq} in vacuum

N	1.42639671511010	-0.07660960925191	-1.34935685135418
C	1.41691090128120	0.15436268184627	1.03511350486142
C	0.73635772463320	0.02074318165570	-0.19974565409102
C	3.54267315518433	0.23629916994624	-0.21429267831665
C	0.69686185662118	0.10600618735727	2.26521744351710
C	2.83313103082021	0.34279876340635	1.03136798366798
C	2.81483123280086	-0.04562605072434	-1.40530048362483
C	3.48500209237978	0.58550384181332	2.25515346593424
H	4.55964699450216	0.75742759053111	2.28503956206798
C	4.94722881424354	0.34378201981602	-0.30120174666676
H	5.52889790633147	0.57405143999550	0.59012624619109

C	1.38997576894851	0.34482465287430	3.44282015434990
H	0.86897423905864	0.34671684029541	4.40007985980532
C	4.87898192626111	-0.18818288761740	-2.65156953892457
H	5.40320475977386	-0.37572068149417	-3.59091203062053
C	3.50380568114235	-0.28160439187190	-2.61389389947505
H	2.98476286243147	-0.55827818877906	-3.52890525642643
C	5.60640258170690	0.14383814264696	-1.49427031332247
H	6.69402552983891	0.22788627352682	-1.53868666807826
C	2.76909403510560	0.60129627595808	3.43404000704240
H	3.28227010589653	0.79935992317498	4.37747226799717
N	-1.40957424477746	0.12979906426181	-1.36443765471727
C	-1.43269398947993	-0.20260879048207	1.00794944360857
C	-0.73536163703714	-0.01658633478380	-0.21063831901928
C	-3.54098899170196	-0.23200140479341	-0.27305940719403
C	-0.72959857446014	-0.20644880831192	2.24877791704768
C	-2.84864099672386	-0.39060583377123	0.97673623463213
C	-2.79704994011011	0.10051925132360	-1.44088456787580
C	-3.51722310162038	-0.68438344478331	2.18014289605859
H	-4.59214158431972	-0.85700231664087	2.18806412719908
C	-4.94406503975023	-0.33667079775503	-0.38394880598736
H	-5.53769151679422	-0.60497035508751	0.48866167981078
C	-1.43878932028340	-0.49456871628670	3.40559129184971
H	-0.93100844746921	-0.53702645302131	4.36899627441034
C	-4.84397225085194	0.29443929286591	-2.70849298172602
H	-5.35536662120906	0.52123558072167	-3.64624696033533
C	-3.46957030113706	0.38709365345210	-2.64781314492979
H	-2.93833932066095	0.70259207043191	-3.54305013488234
C	-5.58692090330508	-0.08684130146683	-1.57651790267345
H	-6.67371134158432	-0.16974070565349	-1.63956454188637
C	-2.81758877337964	-0.74997194947930	3.36705091962621
H	-3.34365638076345	-0.98737500165353	4.29416275156580
C	-0.63021797955218	0.43010554334783	-2.56448275361458
H	-0.47399274211438	1.52036134626985	-2.62088640216916

H	-1.19193124159259	0.11807298423736	-3.44844891122887
C	0.66382067530538	-0.32381059390870	-2.57205733123648
H	1.23771053296410	0.02671447171856	-3.43351914483747
H	0.50882811833697	-1.41049562585713	-2.67857994602914

l-amino-pBiphe (**10**), S_{0,eq} in vacuum

N	1.37391451675050	-0.17217322365230	-1.37375497324376
C	1.46863911797690	-0.03790252373387	1.02926600319870
C	0.76607247363081	-0.08395021860865	-0.22836800317483
C	3.55427267321498	0.05056960672543	-0.28486342999074
C	0.75616209306110	-0.06967226677040	2.25924426559226
C	2.89356974235079	-0.02080040813420	1.00374946160544
C	2.73154123074403	-0.11862043624892	-1.43931525179998
C	3.57512576964958	-0.14628909815294	2.23650378945927
H	4.65768617206813	-0.25237409125766	2.24740050301810
C	4.95194806698790	0.27083772584295	-0.49078247348299
C	1.48137887900137	-0.14754714208759	3.44532349240796
H	0.96864967749762	-0.18893461383056	4.40596186028320
C	4.66190226910282	-0.11243363937268	-2.88526322576231
H	5.11444472215668	-0.19421122100574	-3.87623961324898
C	3.29781470080236	-0.22168047471144	-2.72795946721328
H	2.61405367473729	-0.37186210821605	-3.56366333668660
C	5.47479073011267	0.15659773361024	-1.77901661020596
H	6.54831593277954	0.31024356458802	-1.92068645923236
C	2.87511486170050	-0.21216609481504	3.42627544456903
H	3.42075920477268	-0.32539528039132	4.36598322676300
N	-1.31716953075039	-0.07682384678570	-1.39174650423853
C	-1.42187150701755	-0.04209730882274	1.02087996308958
C	-0.71653238452449	-0.07099894621925	-0.23646539498119
C	-3.49981352211431	-0.03085170338810	-0.29074349155378
C	-0.71687994999513	-0.03778293618115	2.25568062527426
C	-2.84077745758961	-0.01773145353699	0.99570187045022
C	-2.67572273747311	-0.06144011731807	-1.44901485574057

C	-3.54246776935096	0.01859635253106	2.21653392496693
H	-4.63245008100858	0.03897735016304	2.22172138740828
C	-4.90006047144823	-0.01483309711908	-0.45958423152583
H	-5.55471412847582	0.00823451529613	0.41297807365161
C	-1.45605527879829	0.00463786983603	3.43464102436722
H	-0.95228305492511	0.02243760177407	4.40081842061205
C	-4.64517368611784	-0.05909312262379	-2.86692060417234
H	-5.09979542343692	-0.07011669371758	-3.86022779402895
C	-3.27414476894177	-0.07462215407671	-2.73107562921746
H	-2.60249945987492	-0.09795107939585	-3.59092078469753
C	-5.46273724032262	-0.02888515353411	-1.72117579750805
H	-6.54980886019860	-0.01655222818278	-1.82890620043651
C	-2.85444167126682	0.03216074390371	3.41320736393152
H	-3.40421260371011	0.06542977141741	4.35653720175625
N	5.81283572696759	0.58618321735229	0.55374596754869
H	6.71915864508661	0.91171754630205	0.23875131226835
H	5.42366070618871	1.21226908254883	1.25038894992057

2-amino-pBiphe (**11**), S_{0,eq} in vacuum

C	-7.26925469424944	-2.70646982394118	-0.02918614119142
C	-5.89691254967521	-2.58171203928495	-0.03385569079147
C	-5.28708017545242	-1.30489844949807	-0.01849682185873
C	-6.10230211735356	-0.14053380466377	0.00203770562290
C	-7.50391189659922	-0.29772647083797	0.00635522227681
C	-8.07787941541245	-1.55433121726085	-0.00893769008179
C	-5.43251571673625	1.14089650537077	0.01725563738753
C	-4.01291095997558	1.15576080926640	0.01052602780581
C	-3.31598902621403	-0.10913065035839	-0.01103888931691
C	-3.30170650290137	2.38788095950871	0.02475795268386
C	-4.03416690978356	3.57196413597669	0.04543973002999
C	-5.43234067430379	3.55945631789336	0.05211997750979
C	-6.12669467994634	2.36623387532888	0.03831964192892
H	-7.73159041028957	-3.69625957373980	-0.04120431198700

H	-5.23238851665184	-3.44728845233850	-0.04943302765943
H	-8.15135295826966	0.58045202540433	0.02183960592004
H	-9.16583371533100	-1.65271738513004	-0.00536724078997
H	-3.52415651928341	4.53500463839484	0.05678407282821
H	-5.97717389623010	4.50612117842540	0.06839372711307
H	-7.21673198739991	2.37780519583901	0.04380016541740
C	-1.83648116393040	-0.11157951959039	-0.01842194153157
C	-1.12847755571253	1.14420084463441	-0.00321552314789
C	0.12405378770736	-1.31962018946958	-0.04579675933039
C	0.29181078500486	1.12004194441560	-0.01008485306204
C	-1.82881507776293	2.38275056427488	0.01745972784383
C	0.73459330203225	-2.59766847427929	-0.06726822733464
C	0.95596376466072	-0.16554648570974	-0.03091930321457
C	0.99393695174313	2.34083168999473	0.00252701231326
C	-1.08821693461205	3.56132662533599	0.02995552540638
C	2.09942609565199	-2.73503214039054	-0.07345070256776
H	0.07132902855557	-3.46432099123998	-0.07791968993372
C	2.35141181369620	-0.32577257241021	-0.03366117628226
C	0.31018673427449	3.53987263950798	0.02224781610036
H	2.08412064926256	2.34448516556071	-0.00456735183734
H	-1.59178286384991	4.52777578547739	0.04543656804310
C	2.93963006151664	-1.58970761836038	-0.05530721493068
H	2.55369098464846	-3.72932167396055	-0.09515288474756
H	3.00334302884380	0.54984884914508	-0.02149730849704
H	0.86190987738143	4.48255596211569	0.03141839717160
N	-3.92825731404673	-1.25920015299202	-0.02436063428420
N	-1.22863339292149	-1.26567529844049	-0.03892354296609
N	4.30336216879921	-1.74453247119980	-0.10217979226045
H	4.87499986412110	-0.95431560269356	0.16200409123598
H	4.68068872699505	-2.64220465408082	0.16746811496605

3-amino-pBiphe (**12**), S_{0,eq} in vacuum

N	1.36816188778390	0.00314396708378	-1.38348892306618
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C	1.45079458058805	0.01602590067225	1.03288858668204
C	0.75902645375006	-0.00134420448817	-0.23251041129878
C	3.53600867279816	0.04668409442934	-0.26173539002681
C	0.73928244613928	0.00883797122016	2.26423414206244
C	2.87115681693313	0.04121937528085	1.01618591241627
C	2.72867684948548	0.02491607879570	-1.43274536716352
C	3.56331106682505	0.05928630887064	2.24465509310501
H	4.65343806132471	0.07827104007408	2.25775508506499
C	4.93573215611605	0.07317144935822	-0.43279393120745
H	5.59234000606137	0.09213502064821	0.43866972833263
C	1.46866653892183	0.02741327691572	3.44947565250626
H	0.95818678064813	0.02281207810984	4.41225079278008
C	4.70838353325377	0.05429507087000	-2.85812427465897
C	3.32687530893418	0.03059644202083	-2.70783935543208
H	2.65651671301923	0.01378638288138	-3.56936199728692
C	5.50798451704450	0.07587363965834	-1.68508933589355
H	6.59685148854436	0.09026578484143	-1.78294087845815
C	2.86780427751087	0.05238246233938	3.43641386291994
H	3.41209968360504	0.06635169106704	4.38351243041701
N	-1.32392829623330	-0.03881550785626	-1.39657940507728
C	-1.43267638955691	-0.03357126122597	1.01687791698945
C	-0.72425253209810	-0.02552461044408	-0.24076541859776
C	-3.50846501115011	-0.07294128882930	-0.29973024955845
C	-0.73340749731411	-0.01751020895660	2.25576540077393
C	-2.85185463042341	-0.05801924322820	0.98815022079342
C	-2.68219874416524	-0.06203225033083	-1.45637856906958
C	-3.55832209487627	-0.06671529171289	2.20673257756495
H	-4.64830151749856	-0.08551775999249	2.20775226799591
C	-4.90826969876559	-0.09738052473966	-0.47136618572926
H	-5.56486798568745	-0.10622911602356	0.39999763226288
C	-1.47742832695536	-0.02714872701825	3.43228147601734
H	-0.97636558914937	-0.01581211679812	4.39998286367941
C	-4.64861980566590	-0.09974143675568	-2.87850112715555

H	-5.10096784851409	-0.11047137657861	-3.87286506079617
C	-3.27793464215840	-0.07590079633281	-2.73970529683507
H	-2.60424889326910	-0.06711599894669	-3.59823861999941
C	-5.46848552367644	-0.11050010448115	-1.73409992905415
H	-6.55528069507004	-0.12941484000103	-1.84348279703000
C	-2.87556606600311	-0.05158133061887	3.40636989910923
H	-3.42938300797625	-0.05865991495028	4.34790879956039
N	5.30532569273321	0.01269867590319	-4.09613487297174
H	4.72842593663003	0.24818682411977	-4.89198729865197
H	6.25727532755674	0.34529437514933	-4.16269564601481

4-amino-pBiphe (**13**), S_{0,eq} in vacuum

C	-7.19614670673582	-2.76566679951696	-0.02028077932559
C	-5.82537144889555	-2.62560087117320	-0.01478878012035
C	-5.22895697545225	-1.34255644155087	-0.01011091478061
C	-6.05725233607551	-0.18675630889880	-0.01125316672722
C	-7.45693642459054	-0.35977616838174	-0.01666729109621
C	-8.01736429857557	-1.62253283081798	-0.02116438086169
C	-5.40399126033609	1.10351208991751	-0.00747690034771
C	-3.98497312728422	1.13586668192880	-0.00343084947120
C	-3.27447934407481	-0.12056104930406	0.00046547546155
C	-3.28663101950772	2.37609047104312	-0.00268284544934
C	-4.03368997567101	3.5511259777483	-0.00205785859295
C	-5.43172873252580	3.52170768978208	-0.00429666139085
C	-6.11265424201268	2.32060599447035	-0.00777798396998
H	-7.64732064485509	-3.76063439502193	-0.02366546505183
H	-5.15345351759486	-3.48556463474684	-0.01327691772883
H	-8.11379700482347	0.51138833935105	-0.01754596367765
H	-9.10418099295473	-1.73273946684684	-0.02537616936441
H	-3.53507399130005	4.52020876691517	0.00058353961991
H	-5.98764952182015	4.46202572579592	-0.00356976348086
H	-7.20278794988563	2.32013214896115	-0.01032131304249
C	-1.79781306063836	-0.10043426482771	0.01161306633851

C	-1.10048531014980	1.15786787928912	0.00422791277599
C	0.17866340298947	-1.28929107570548	0.03242373583883
C	0.32068657487670	1.14176035115871	0.00246523475669
C	-1.81368154781226	2.38889849458330	-0.00413402629432
C	0.75752786691253	-2.60649014127504	0.05188146017362
C	1.00306556172398	-0.13470635099812	0.01167033182944
C	1.01117627048011	2.36959900954000	-0.00776854091848
C	-1.08348876170039	3.57358800053324	-0.01483289159060
C	2.14839206300757	-2.71769773138539	0.03065771833697
C	2.40162521127946	-0.29227873049904	-0.00170248317739
C	0.31562220021903	3.56209300798547	-0.01627625664940
H	2.10126260916754	2.38027773043532	-0.00809742086275
H	-1.59442365032496	4.53633245709187	-0.02307141825188
C	2.94506795451504	-1.56759656486848	0.00428957709619
H	2.61303024493915	-3.70643869983517	0.03996531182704
H	3.06193272352102	0.57453455955318	-0.01987176121899
H	0.85944921655742	4.50937771403419	-0.02429834813263
H	4.03186420652762	-1.68355310119316	-0.01016472175372
N	-3.87024722507402	-1.28042132815325	-0.00380021850934
N	-1.16948071205995	-1.24341382888425	0.02714093589466
N	-0.09537914876132	-3.65341077010429	0.10418032037605
H	-1.08204431021897	-3.42508621194328	0.03112188144448
H	0.22781713499511	-4.59688532421249	-0.03402440993060

8-amino-pBiphe (**14**), $S_{0,eq}$ in vacuum

N	1.34721938540994	0.13521515314189	-1.36942405806119
C	1.45911846696194	0.05819175098405	1.04798377763530
C	0.75282006797356	0.05697045415788	-0.21212060199791
C	3.52815891188403	0.17902607833225	-0.28214501611856
C	0.75042158426910	0.00436299877751	2.28527175096399
C	2.87475713949910	0.06764558636137	0.99725836971439
C	2.69975543191736	0.22163877742281	-1.43700448409080
C	3.58203958835273	-0.04741790511401	2.21204797401320

H	4.67226010215655	-0.03607832713653	2.21774131849342
C	4.92756871898231	0.25058444275652	-0.45533237786922
H	5.58811832528409	0.22171014165005	0.41280497086179
C	1.49555745184936	-0.23030367292414	3.46132786470894
C	4.65696437634222	0.41358263434620	-2.85790976019267
H	5.10611389037184	0.50582286260683	-3.84941752536620
C	3.28879455405269	0.33967718005608	-2.71868744396209
H	2.61219583207900	0.36639321565598	-3.57462397494483
C	5.48014063732479	0.36753537872482	-1.71536390735520
H	6.56554778486212	0.42603591326319	-1.82587880096695
C	2.90998425420831	-0.21960792374390	3.39378674961527
H	3.47167926567295	-0.35861916596410	4.32173224268860
N	-1.32036175397097	-0.24234979560757	-1.35614124431291
C	-1.42249728991791	0.04817572992040	1.04139197124596
C	-0.72145221936893	-0.07278667552819	-0.21140487661149
C	-3.49981028395589	-0.11208249524750	-0.25962456869790
C	-0.71108813677675	0.17155768552458	2.27237055726060
C	-2.84029506203941	0.09877944573591	1.00903553584047
C	-2.67736761104515	-0.29824532680430	-1.40448423166339
C	-3.54259972496209	0.36665512542137	2.20124274556875
H	-4.63137334528128	0.41993879294196	2.19753706483833
C	-4.90080365671223	-0.15166680327553	-0.42141574478243
H	-5.55362489240033	-0.01220041107387	0.44167545535570
C	-1.45195997087536	0.50142362594704	3.41080985476120
H	-0.94309899386251	0.73256844163530	4.34492072501707
C	-4.64959508283470	-0.56917652567812	-2.79273537099256
H	-5.10586341254265	-0.74708873830266	-3.76932641393801
C	-3.27852660591194	-0.52735356019261	-2.66505748203456
H	-2.60880763446102	-0.66250741003393	-3.51607839607352
C	-5.46580704348889	-0.37799377910311	-1.66128345063605
H	-6.55303367151263	-0.41009730615292	-1.76318884603513
C	-2.84838963776700	0.60253038341902	3.36867108773487
H	-3.38969091150432	0.86708187608770	4.28016451989757

N	0.92813976362570	-0.45980477870191	4.69726308245683
H	0.00908304042094	-0.88664323417563	4.69666736208376
H	1.55380836769127	-0.87437984011018	5.37634359594752

9-amino-pBiphe (**15**), S_{0,eq} in vacuum

N	1.35486007293189	0.05121188700761	-1.43150867526940
C	1.46823537836163	0.06992588972593	0.98050815250513
C	0.76179311183668	0.03780197533954	-0.27074177661858
C	3.53997923126497	0.13408362457758	-0.33105831119982
C	0.78070614935960	0.05334799431792	2.22577053124823
C	2.88746086882910	0.11738889361570	0.96088390519250
C	2.71269768784134	0.09871674467959	-1.48741813508666
C	3.59730899441161	0.14176111054599	2.16969849833123
H	4.68758665560086	0.17729260158297	2.16442112725667
C	4.93873644617301	0.18385177769689	-0.50421871160211
H	5.59485646671431	0.21373724056675	0.36716528758629
C	1.51952661785992	0.08053635502276	3.39817081777684
H	1.01736785320431	0.07305085033297	4.36642869139328
C	4.68058643537350	0.16135939905093	-2.90981651927746
H	5.13195016623159	0.17235449831821	-3.90471135050918
C	3.31068704262233	0.11307349065223	-2.77016217284890
H	2.63776350596989	0.08457302841966	-3.62891329394775
C	5.50058133424087	0.19729204556117	-1.76621137340198
H	6.58687946670322	0.23656993228253	-1.87555677185420
C	2.93066269288455	0.12353286813903	3.39267746804777
N	-1.33783850647341	-0.04594563270309	-1.40210894442820
C	-1.40956869513072	-0.02712363517468	1.01249802990157
C	-0.72048714330181	-0.01445508047992	-0.25650441299916
C	-3.50461494548234	-0.10856215620735	-0.27207447130751
C	-0.69287767553015	0.00690803112831	2.24112300498616
C	-2.82836015629475	-0.07395043126376	1.00532889376012
C	-2.69644516525588	-0.09269596816195	-1.44119258548678
C	-3.51663627438774	-0.08466373153989	2.23433214140123

H	-4.60610206112785	-0.12008280348372	2.25127770928589
C	-4.90626025890597	-0.15687603714780	-0.42191986063173
H	-5.54962361993051	-0.16978263976301	0.45922204447593
C	-1.41937867468929	-0.00429437456080	3.42810546609000
H	-0.90553322499923	0.02347754069969	4.38880780484916
C	-4.68305863020676	-0.17308217676851	-2.83264612166586
H	-5.15016264492301	-0.19840979357472	-3.81989513678288
C	-3.31094680161367	-0.12583377920161	-2.71510037253606
H	-2.65052042392639	-0.11197902784072	-3.58380122245575
C	-5.48519324165683	-0.18857693234095	-1.67591356935054
H	-6.57309418642900	-0.22586960605269	-1.76860746227882
C	-2.81724937836039	-0.04964380248818	3.42370013719085
H	-3.35715025785564	-0.05699791817222	4.37327619211325
N	3.61526518619419	0.18840558425243	4.58055668142713
H	3.13398872723461	-0.10811365579433	5.41775773450594
H	4.60252187463728	-0.02541418079653	4.56567093221412

10-amino-pBiphe (**16**), $S_{0,eq}$ in vacuum

C	-7.21298210379603	-2.71672908194275	0.22466904396822
C	-5.84264651762058	-2.57384662029638	0.23311388612973
C	-5.24916496124577	-1.29334276094949	0.12971739563258
C	-6.07835825641667	-0.14371903693361	0.01646356355673
C	-7.47784626605911	-0.31992704454376	0.00864201468346
C	-8.03544340203124	-1.57966406450666	0.11093635021998
C	-5.42600035498020	1.14247744900091	-0.08137831884629
C	-4.00716048781819	1.17463725907721	-0.05003360852775
C	-3.29624948854569	-0.07408306661126	0.05398991188782
C	-3.30394848345145	2.40844859930298	-0.12352209891170
C	-4.04789790756377	3.57944357539274	-0.25316085198348
C	-5.44536431201032	3.54958117861034	-0.29441614326181
C	-6.13207255255058	2.35467864046401	-0.20528786578644
H	-7.66329606093292	-3.70884509604736	0.30502836157090
H	-5.16748801093302	-3.42712062842430	0.31751359070669

H	-8.13557195114045	0.54636927584045	-0.07744675954229
H	-9.12202451483474	-1.69287720375905	0.10364403725261
H	-3.54755798224652	4.54484808118535	-0.32922293223317
H	-5.99737155428009	4.48670205173431	-0.39759701375966
H	-7.22176613434421	2.35510215548691	-0.23521187441822
C	-1.81193877812408	-0.06503858236763	0.04634725180231
C	-1.10899288514767	1.19685772668755	-0.00949670621055
C	0.14316280416054	-1.27527822186125	0.03204469446851
C	0.31505400438872	1.17324903346303	0.02563261861817
C	-1.83743324184779	2.41524422696289	-0.05742196247773
C	0.72122939316211	-2.56530782869424	0.00367753924040
C	0.96920845674060	-0.11696149989870	-0.06906810993230
C	1.00683401225518	2.41525112837535	0.17837961711787
C	-1.10824680911970	3.60118435087856	-0.02377724490893
C	2.07620877272165	-2.73084196952476	-0.18318193528517
H	0.03784074716774	-3.40973911306311	0.10833153108228
C	2.34844110799390	-0.32522096755509	-0.31769620635548
C	0.27253373739929	3.60030091854992	0.11344924198402
H	-1.61810320403797	4.56399996887847	-0.05914126501651
C	2.88588295838970	-1.59884773623218	-0.37361567786390
H	2.51315165562229	-3.73152085090582	-0.21335920411644
H	2.99560944584805	0.52235452566414	-0.53531457033835
H	0.80329936923017	4.55194610748864	0.20348107336996
H	3.95153431868502	-1.72001467040295	-0.58250085435237
N	-3.89103989464160	-1.22999354224318	0.13857907769801
N	-1.21030128175095	-1.21601229931259	0.11507293654419
N	2.36902545153239	2.48611847116258	0.38375081984676
H	2.69707947168859	3.39031829204886	0.69946685223286
H	2.77907169048565	1.72101886982083	0.90601979451448

2,10-diamino-pBiphe (17), S_{0,eq} in vacuum

C	-7.22696495212107	-2.70727760066578	0.20761394789882
C	-5.85615372746305	-2.56899625456808	0.23174694833713

C	-5.25546498693044	-1.29176036959920	0.12759848310069
C	-6.07997180883757	-0.14075367891009	-0.00277536417261
C	-7.47983427377513	-0.31188255204937	-0.02621044540349
C	-8.04437824338339	-1.56860183931781	0.07703534610279
C	-5.42190688378566	1.14300855461027	-0.10101431100639
C	-4.00327636578050	1.17076614365978	-0.05328614305609
C	-3.29623822092456	-0.08014914295533	0.06774967745072
C	-3.29585790981339	2.40244013989380	-0.12676591450902
C	-4.03528488158851	3.57517428002612	-0.27223151230808
C	-5.43170903894410	3.54898553316703	-0.32925178797103
C	-6.12276561360374	2.35621005376620	-0.24068290762348
H	-7.68131317920068	-3.69760647417155	0.28873793594607
H	-5.18535860365135	-3.42430881733127	0.32972679785971
H	-8.13287840973518	0.55663751769247	-0.12559623833844
H	-9.13126213509724	-1.67765818777070	0.05729318975294
H	-3.53123999492847	4.53861613765258	-0.34886784950921
H	-5.98006640429054	4.48690406442833	-0.44474684045249
H	-7.21207396176204	2.35936889746329	-0.28338123465861
C	-1.81535242063316	-0.07146039807612	0.07882822788108
C	-1.10685624063406	1.18513870933463	0.01936856256580
C	0.13811057920472	-1.28135860618813	0.10117071989591
C	0.31809071935822	1.16060341624835	0.06692112765063
C	-1.83016030712375	2.40657375625420	-0.04501060222217
C	0.72742115770947	-2.56840472804083	0.09730567079579
C	0.97465794591910	-0.13049478027666	-0.01159296509132
C	1.00893208452250	2.40265124358893	0.21766561803308
C	-1.09933143639812	3.59140719357550	-0.01228910187549
C	2.07698950104180	-2.74066478995343	-0.07657364057205
H	0.05089801346671	-3.41683567954233	0.21410811652084
C	2.35258902737728	-0.33483891410212	-0.23790379883531
C	0.28021933096485	3.58978647280075	0.13868271880813
H	-1.60763504633914	4.55459599511093	-0.05987211655408
C	2.91172992338259	-1.61398025066979	-0.28538539339493

H	2.51099141052758	-3.74396673602171	-0.09292762428938
H	2.99920883933087	0.51095753566942	-0.46825749713593
H	0.81262908356518	4.54058515837534	0.22830025702524
N	-3.89735503001219	-1.23384134411120	0.15282440230452
N	-1.21027691893403	-1.22242097582022	0.16679913809105
N	2.37082609687680	2.47047711937354	0.44032045991129
H	2.68887085044727	3.37293049211942	0.77171583270049
H	2.76025134106051	1.70356314548314	0.97666620617449
N	4.23978177545313	-1.79355278335959	-0.57802510743602
H	4.85937998964808	-1.00009725591009	-0.50033189908745
H	4.65768932583460	-2.68786940088266	-0.36569908930411

[2-amino-pBiphe-H]⁺ (**18**), S_{0,eq} in vacuum

N	1.30508264783736	0.01728036796528	-1.39610028522763
C	1.45216396008399	0.04286164965710	1.02664867636297
C	0.73661155200059	0.01382805929176	-0.20802445619935
C	3.50000656997206	0.08175979789193	-0.33602178003573
C	0.75806860176698	0.03671867959450	2.26696158865269
C	2.86775091369091	0.07770612768943	0.96889013491231
C	2.64188716759362	0.04987037390172	-1.48959956995860
C	3.58407518800907	0.10650774530562	2.18055381326276
H	4.67386207308829	0.13359910290384	2.17634016525990
C	4.88113822547034	0.11465281431725	-0.52458013855513
H	5.55169955846814	0.13918002905092	0.33537058234707
C	1.51474922735463	0.06620963266073	3.43552452664571
H	1.02779187862565	0.06292233235498	4.41087384722497
C	4.58301970665547	0.08530981149922	-2.94731667744090
H	5.02016884680002	0.08721043359097	-3.94855219148829
C	3.22864767456493	0.05285936471180	-2.78558231090906
H	2.55737288443758	0.02834173088167	-3.64551857905991
C	5.44696829942687	0.11721927770243	-1.80930567880876
C	2.91325388100739	0.10070767139031	3.38943664350185
H	3.47819610864349	0.12325055574949	4.32327874265830

N	-1.34936097220239	-0.04843290581915	-1.33870408364758
C	-1.42736542755368	-0.02895027755552	1.04191183123458
C	-0.70534717273487	-0.02192086427769	-0.17852937744485
C	-3.51042055079345	-0.09300721294763	-0.30124470132860
C	-0.71123882483307	0.00003349141308	2.27503095124722
C	-2.85095074613667	-0.06491385540942	0.99434467384188
C	-2.71683224258655	-0.08376811511455	-1.47334554193685
C	-3.54993654752926	-0.07144546321412	2.20968109710839
H	-4.63900993585794	-0.09847066607034	2.22237679837173
C	-4.90819760170209	-0.12932825476820	-0.46746047480749
H	-5.55737377520436	-0.13761577365551	0.40810558865332
C	-1.46100354282719	-0.00818904556460	3.44871135531782
H	-0.96748059989384	0.01280026850391	4.41994669443969
C	-4.66870157521910	-0.14501609520725	-2.87467925319596
H	-5.12508596990885	-0.16531439737070	-3.86619367191345
C	-3.29320057690081	-0.10963830241900	-2.75222605412236
H	-2.64982027750973	-0.10155195152175	-3.63496848975740
C	-5.47793934673032	-0.15484898760804	-1.72727028112262
H	-6.56427982177581	-0.18279952600520	-1.82953722321102
C	-2.85734205356976	-0.04341261528962	3.40999176605741
H	-3.41422240134413	-0.04890030646474	4.34944490098723
N	6.78183838029096	0.14867081103105	-1.98783439382770
H	7.18386008904608	0.15214156960447	-2.91386153385608
H	7.41565968231165	0.17349833897216	-1.20233708109537
H	-0.73346315433223	-0.04051542135260	-2.15763054913709

[10-amino-pBiphe-H]⁺ (**19**), S_{0,eq} in vacuum

N	1.32403545140771	0.15905777765051	-1.32962080725408
C	1.46951263542202	0.05014808571078	1.09336594408465
C	0.76540510679949	0.07596870382275	-0.15118079814550
C	3.51453546722304	0.05961119359016	-0.26287553256212
C	0.74583631621899	-0.03201890627622	2.30993715528014
C	2.88875656914062	0.13277856500197	1.03759218153356

C	2.67240207363606	0.13166778873075	-1.42357866588109
C	3.59127560680030	0.29565775651954	2.28158843578609
C	4.89783002180589	-0.14162157536809	-0.49377389627661
H	5.56710030153824	-0.34496732867890	0.33971008923040
C	1.49358286151274	-0.01369260527458	3.48997610736526
H	1.00051223276490	-0.09326855948498	4.45916484938079
C	4.58935727798829	-0.00350913081014	-2.90106699525481
H	5.01999735246673	-0.01286828663119	-3.90411560482372
C	3.23337846852675	0.13110410476392	-2.72388240840231
H	2.54655016812938	0.21319389038699	-3.56779324472617
C	5.41620149262858	-0.17380489213417	-1.77402975214887
C	2.86711768396564	0.15890267200066	3.47494054812376
H	3.40558916434605	0.23238439987497	4.42266631694516
N	-1.31007946787796	0.07405086409660	-1.30730083116410
C	-1.42105443269008	-0.07723613456968	1.06317990663206
C	-0.69018545989018	0.02794431018854	-0.13695272569342
C	-3.48394596272692	-0.08362522759474	-0.30884194479740
C	-0.71169625881298	-0.11998754626734	2.30263109032959
C	-2.84651095076283	-0.14174266646319	0.99514982954853
C	-2.67409513991163	0.02747718747748	-1.46572588345941
C	-3.55630725719640	-0.25942882368468	2.19541463179126
H	-4.64429762618644	-0.31418142762850	2.19615228150068
C	-4.87876261112953	-0.13163280598524	-0.49993315386862
H	-5.53990205840764	-0.21632980542706	0.36247850956153
C	-1.47745347690355	-0.24170701888853	3.46266740477241
H	-0.99724966075956	-0.28640597654373	4.43976560659210
C	-4.60296716194324	0.03760377156546	-2.89858655736592
H	-5.04524034254224	0.08380455664944	-3.89559113470853
C	-3.23090590148688	0.08746702751888	-2.75270902260306
H	-2.57500258424040	0.17276414727038	-3.62203777315427
C	-5.42836178730361	-0.07224597875145	-1.76690663268597
H	-6.51242587371933	-0.11094495407269	-1.88866878541997
C	-2.87037490939173	-0.30998739097826	3.40163879365928

H	-3.43535268971366	-0.40486962069074	4.33161847805443
H	-0.67796780165000	0.14535774841337	-2.11189041269179
H	6.48565259347062	-0.34897940466047	-1.91076855984941
N	4.92014525259963	0.57619894134996	2.34449271989320
H	5.35975677025881	1.04826065263566	1.56608462972751
H	5.29870854659633	0.81345192164578	3.25241561314475

[2-amino-pBiphe-Me]⁺ (**20**), S_{0,eq} in vacuum

N	1.38503771573286	-0.06815148316778	-1.41287188866985
C	1.46820350270954	0.17429139425496	0.98639184314918
C	0.76165926359901	0.10697258626877	-0.26239736669443
C	3.55701115714764	0.03728063371273	-0.31443303639502
C	0.76936556622611	0.20390817865645	2.21806665190598
C	2.88759250136693	0.18654100129022	0.96068565981154
C	2.71976389634987	-0.12667678084680	-1.46740025932841
C	3.58390384003639	0.31451184884492	2.17617369559103
H	4.67368775870099	0.33790663315896	2.18377246845535
C	4.94135949813818	0.01956797737135	-0.47385629092308
H	5.59733887470065	0.14943592354159	0.38790859249529
C	1.50276631556296	0.33591599557755	3.39639554278399
H	0.99746590213771	0.38314192634937	4.36079213287163
C	4.68636800678865	-0.35946562841196	-2.87366161270358
H	5.14221197405266	-0.51790693818920	-3.85381251952283
C	3.32927350633296	-0.33494559612467	-2.73777280955880
H	2.67229523589853	-0.47069229187340	-3.59840975252466
C	5.52963831551186	-0.17462841242264	-1.73427410880242
C	2.89760285011791	0.40505789004473	3.37279173446450
H	3.44700619622705	0.51282582151957	4.30988086423728
N	-1.38671436776420	0.35581132094789	-1.40954834839292
C	-1.39580784963694	0.00119397496434	0.96833498560060
C	-0.69189147035612	0.16378393049423	-0.26760007174519
C	-3.48294546966081	-0.23355862464160	-0.32103461847672
C	-0.68537320164685	0.04891385866798	2.20711839950974

C	-2.80978495042778	-0.15423244274269	0.95763783957472
C	-2.74768456947746	0.04182844264558	-1.49513879072475
C	-3.49720369851083	-0.24476394301743	2.17479603584440
H	-4.58140429340508	-0.34720967787814	2.18870497504126
C	-4.84585304760834	-0.56447887793745	-0.44568974886754
H	-5.42608631799234	-0.79471029490641	0.44738225659243
C	-1.41836086675694	-0.05171166091567	3.38840922534071
H	-0.91011644582015	-0.02299266959565	4.35124805294220
C	-4.72170976216897	-0.35198601937688	-2.83763183065225
H	-5.19471565232118	-0.41495883884456	-3.81958508032743
C	-3.38173103025126	-0.02274856605732	-2.75050388246105
H	-2.82180112415886	0.14930144351638	-3.66723625488131
C	-5.46262992641100	-0.62030911529665	-1.68001735249373
H	-6.51923189113444	-0.88414649741747	-1.75197661163852
C	-2.80455675996561	-0.19370533455158	3.37215780632215
H	-3.34848738509503	-0.26520550676804	4.31627721517866
C	-0.78750548818130	0.98409686463941	-2.58915402236837
H	0.08120511084223	1.57123315844111	-2.28758347182290
H	-0.45859011542770	0.24103957834052	-3.32563773750353
H	-1.54098810865123	1.64983143398438	-3.02626177085805
N	6.86752525711249	-0.19327530167151	-1.88710166908472
H	7.28650525657603	-0.34064640092337	-2.79373617066415
H	7.48718629096121	-0.06948491365411	-1.09959889962642

[10-amino-pBiphe-Me]⁺ (**21**), S_{0,eq} in vacuum

N	1.40728706861652	-0.01666390845192	-1.35670358285298
C	1.48853541763869	0.14398366696107	1.05186390876943
C	0.79524618828811	0.11855044909369	-0.20801809711348
C	3.57015880819045	-0.06713480773330	-0.23048639168603
C	0.76045658945093	0.11026988794929	2.26143914736989
C	2.91133253902965	0.19725639972803	1.02515930149109
C	2.74840414361662	-0.15895190427347	-1.40068180621156
C	3.58936620060253	0.48332397164819	2.25936382419416

C	4.95134512618038	-0.33561268990197	-0.39577467156657
H	5.60481625903360	-0.40106635812812	0.47165285438207
C	1.48069955956266	0.24417826454532	3.45263359845252
H	0.96820214066606	0.22722481700991	4.41461176066470
C	4.67670894163104	-0.62971647904758	-2.79438690152811
H	5.11936721151955	-0.83695215744695	-3.77047602091895
C	3.32493664424728	-0.41851704138147	-2.66935750445766
H	2.65137737267711	-0.46467566346515	-3.52654431420645
C	5.48388356715318	-0.61153894348181	-1.64045743007745
H	6.54974064374341	-0.83554774862438	-1.72426195409234
C	2.84695368939062	0.45764074719528	3.44883292963419
H	3.36591803301109	0.63123648390155	4.39434404096844
N	-1.34468344723151	0.45656874044997	-1.36102400657799
C	-1.38187623061047	-0.07289040631465	0.98064186135958
C	-0.67252857946326	0.18990019889523	-0.22368937114336
C	-3.45114133976631	-0.22410624624918	-0.34553025856405
C	-0.67729043325733	-0.10092039557604	2.22696182975775
C	-2.79642933411989	-0.24911777598512	0.94351647613702
C	-2.70490301002154	0.15345823636262	-1.48530202977324
C	-3.48934717623854	-0.45633582829159	2.14026733729945
H	-4.57094155947658	-0.58275414974404	2.13921418119719
C	-4.81213438668223	-0.54675664372868	-0.51312652532550
H	-5.40035939774574	-0.85309188654064	0.35131372693728
C	-1.42030463170930	-0.31947269691365	3.38850993772240
H	-0.92147158708465	-0.36114511657793	4.35598629114062
C	-4.66401955616807	-0.12752984056095	-2.87675573594531
H	-5.12749456692492	-0.10642367020610	-3.86500213857829
C	-3.32688413535463	0.19674755938135	-2.74829648703071
H	-2.75975923571069	0.44952095538015	-3.64145604503990
C	-5.41551132899454	-0.49743971330609	-1.75353435775778
H	-6.47052622588908	-0.75636451954745	-1.85918945050598
C	-2.80085123803723	-0.49369608382630	3.34345928483599
H	-3.34939049760436	-0.66022916707205	4.27301061643474

N	4.91747942093775	0.77052659506977	2.31436300422768
H	5.36805069701235	1.16867570432779	1.50160138068231
H	5.28532795710044	1.08820945803296	3.20180980991848
C	-0.72545023960783	1.15988480901572	-2.48812715789714
H	0.15189943100157	1.70756527474052	-2.14223307481730
H	-0.40830983544306	0.46535106696185	-3.27526078560388
H	-1.46398567715986	1.87017855572637	-2.87778100430492

2-dimethylamino-pBiphe (**22**), S_{0,eq} in vacuum

N	1.23739617545796	-0.12652041786682	-1.54062890555487
C	1.42249500117013	0.15787207489689	0.84793035550573
C	0.67095576093237	-0.01507790061778	-0.37041756881652
C	3.45815394262635	0.08373192843149	-0.53623747967344
C	0.76666294959225	0.27575473406881	2.10526466002073
C	2.83992432503588	0.20889668604278	0.76728358587501
C	2.58587822544317	-0.08174365539032	-1.64677265451050
C	3.58305615332212	0.37840378904051	1.95127023648098
H	4.67187824232565	0.42033619383347	1.91209989923139
C	4.84562310161932	0.11764450290401	-0.74537217143347
H	5.50343427474611	0.24382410654652	0.11118913583360
C	1.54720985478142	0.44223292726068	3.24592843059116
H	1.07829765565374	0.53656721173144	4.22525032328907
C	4.51361320091996	-0.17237266986325	-3.12887285751746
H	4.90715678619198	-0.27297594950857	-4.13969347160601
C	3.15577665434339	-0.20717903570647	-2.93584620901955
H	2.46643357961749	-0.33340288723703	-3.77262841067047
C	5.40287270207291	-0.00687629553013	-2.02583596964393
C	2.94252522944667	0.49299022643391	3.16887727297544
H	3.52666954001888	0.62463588710454	4.08246425292275
N	-1.45808861897063	-0.22696562779838	-1.42639040738721
C	-1.45729489512904	0.04986815119950	0.97449332688986
C	-0.80581623295695	-0.07049056600486	-0.30909916921527
C	-3.58933166683905	-0.17994389027530	-0.22868669404961

C	-0.70373696169817	0.21967985438468	2.16924156798915
C	-2.87529251821694	-0.00575836302057	1.01658602946794
C	-2.81638062779429	-0.28386650704964	-1.41720491920838
C	-3.52528229263622	0.10996754523057	2.26066426087318
H	-4.61335910094392	0.07047670211359	2.31552163915060
C	-4.99436121937998	-0.25180686483094	-0.32842352840319
H	-5.60972468646256	-0.17486813159125	0.56936927322190
C	-1.39348993239224	0.32831992361686	3.37411704963934
H	-0.85027168159197	0.45836102341238	4.30990396361969
C	-4.84539403295944	-0.52211946999689	-2.72891627483332
H	-5.34201546917185	-0.65459090397972	-3.69300944438462
C	-3.47074769872838	-0.45519822336459	-2.66017462632225
H	-2.83790564840880	-0.53021943006470	-3.54614572992038
C	-5.61210103430069	-0.41948710194548	-1.55279378708108
H	-6.70193359355310	-0.47257375895094	-1.60677644551414
C	-2.78992396138375	0.27400706252100	3.41757750725785
H	-3.30055483169311	0.36270380323642	4.37920049098471
N	6.76052385038017	0.02790745905910	-2.22295404234918
C	7.30811612705383	-0.10861864397780	-3.54742322903869
H	6.96796545041828	0.69422796327623	-4.22572170987021
H	8.40207562713794	-0.05447355050018	-3.49279915194562
H	7.04458970210544	-1.07544212164078	-4.01265488132849
C	7.63979334201217	0.19212296223714	-1.09721877330400
H	8.68006056032185	0.20015057970881	-1.44403454973959
H	7.45570813953741	1.14166676915678	-0.56226322489501
H	7.53506055092615	-0.62887810073572	-0.36433697458361

[2-dimethylamino-pBiphe-H]⁺ (**23**), S_{0,eq} in vacuum

N	1.22342871663171	-0.11781068777943	-1.49852025927674
C	1.43631641940225	0.16333410693232	0.90410948102878
C	0.68707271851011	-0.00446108689786	-0.29944695087398
C	3.44557152163528	0.08658711138824	-0.51514705308601
C	0.77654481305511	0.27779997799644	2.15786626177319

C	2.84919291322503	0.21102303097752	0.80211976258887
C	2.55540529102672	-0.07711863621493	-1.63194339354919
C	3.59676039600612	0.37640407624043	1.98298538542859
H	4.68552355961715	0.41765810991861	1.94488336312637
C	4.81967426461019	0.11804699441619	-0.74262025381016
H	5.49022034172285	0.24175262067087	0.10361095036460
C	1.56407323853745	0.44011110980463	3.29511654592451
H	1.10370542639435	0.53258642518242	4.27895759371037
C	4.46041684495159	-0.16794769065670	-3.13881906163884
H	4.84524131266186	-0.26609833503344	-4.15253778818803
C	3.11171623513085	-0.20115009759503	-2.93414815298446
H	2.42046492879287	-0.32435108760160	-3.76956070401562
C	5.36563048352252	-0.00584579244794	-2.03799875394960
C	2.95955309726075	0.48852056624805	3.20522539336681
H	3.54956689541364	0.61663107503918	4.11475323092347
N	-1.42695606971852	-0.21310080907839	-1.35745122211308
C	-1.43970386617031	0.05463934607559	1.01015822897015
C	-0.75099172864383	-0.05632828880501	-0.22501340376601
C	-3.55759831676123	-0.17791452991498	-0.25827703919533
C	-0.69093203905363	0.22203778414917	2.21222228058296
C	-2.86312311316343	-0.00553704417410	1.00799791918808
C	-2.79678817030417	-0.28072546411360	-1.44737903656959
C	-3.52834500700971	0.10528788485621	2.23690737466272
H	-4.61607716913625	0.06482299012133	2.28372453121306
C	-4.95850341907467	-0.25012006427417	-0.37887687957363
H	-5.58283143763079	-0.17524355070272	0.51149479989130
C	-1.40819816319625	0.32601573247019	3.40199762802589
H	-0.88845214626790	0.45474397544573	4.35099013036848
C	-4.78596123243445	-0.51465324844566	-2.77695325963314
H	-5.26902851380030	-0.64478399634388	-3.74727946803680
C	-3.40824210467908	-0.44810582270014	-2.69897070494042
H	-2.78975657683070	-0.52373022590062	-3.59618593096450
C	-5.56286501957358	-0.41512346742173	-1.61188046598013

H	-6.65102190673406	-0.46812303970292	-1.67865721250867
C	-2.80390893503761	0.26790950163578	3.40765487465408
H	-3.33492261734811	0.35275638890633	4.35819855829432
N	6.70298070167574	0.02614275551710	-2.24755477568047
C	7.24622046902333	-0.10276552428479	-3.58372767392473
H	6.90452399028349	0.71055481813399	-4.24477980501320
H	8.33918276404746	-0.05486754930479	-3.53230152850668
H	6.97328528734620	-1.06586267091361	-4.04528819035046
C	7.60721875817175	0.19164432365283	-1.13164275254699
H	8.63934187947959	0.19429340871065	-1.49784705774334
H	7.43187567289773	1.14470633825120	-0.60480798869609
H	7.50799687140909	-0.63058434675238	-0.40312747679353
H	-0.83409825987429	-0.28275739568057	-2.19013005017716

[2-dimethylamino-pBiphe-H]⁺ (**23**), S_{0,eq} in chloroform

N	1.22671942828139	-0.12134185054227	-1.50165761687337
C	1.43532171022939	0.16168530948080	0.89873935593427
C	0.68558782537894	-0.00829531174830	-0.30559175056421
C	3.44884081234267	0.08404304854304	-0.51747482621367
C	0.77634832651207	0.27878117415507	2.15303901527899
C	2.84906030300549	0.20978518422720	0.79893445281632
C	2.55941762134246	-0.07985382255834	-1.63406583852505
C	3.59787494039236	0.37790501494487	1.97911901022644
H	4.68700082008431	0.41838011283516	1.94028043271730
C	4.82382318047931	0.11633199482264	-0.74119103139414
H	5.49377679681688	0.23979783263497	0.10613654085079
C	1.56300880913860	0.44673043943432	3.29082521674669
H	1.10220028881261	0.54476653119911	4.27407163934794
C	4.46624402410012	-0.16722227803861	-3.14044731780152
H	4.85280427139374	-0.26347196278685	-4.15417669131441
C	3.11668819729583	-0.20203977489095	-2.93630606591382
H	2.42726661216402	-0.32476728760247	-3.77423303667463
C	5.37058719871115	-0.00639654147963	-2.03772920715072

C	2.95875197900123	0.49446941456600	3.20044509561693
H	3.54835456936145	0.62606580566878	4.11022346791885
N	-1.43403893476448	-0.21725178690503	-1.35932963441454
C	-1.44083377667437	0.05395792204110	1.00640879868683
C	-0.75422083227098	-0.05952387913090	-0.23184405825450
C	-3.56256241579872	-0.17663288297974	-0.25499965110490
C	-0.69162062797693	0.22050084300097	2.20817001674320
C	-2.86422001105564	-0.00465917434469	1.00900147256216
C	-2.80271500822364	-0.28245279416736	-1.44393203735645
C	-3.52855580262508	0.10547254548050	2.23944807476314
H	-4.61668556019505	0.06746833473319	2.28730630438762
C	-4.96459257381704	-0.24577682111512	-0.37342532797228
H	-5.58858921266464	-0.16972900203923	0.51745770234956
C	-1.40534876150598	0.32011398850212	3.40097206823848
H	-0.88358736403276	0.44351631941413	4.34992610621327
C	-4.79145711284816	-0.51335594291564	-2.77338353674079
H	-5.27531486270349	-0.64348050917829	-3.74385450204799
C	-3.41352000253978	-0.45080477724721	-2.69650040332363
H	-2.78866713917250	-0.52899372093965	-3.58904499496013
C	-5.56814799524838	-0.41023478468537	-1.60749708870743
H	-6.65698214679091	-0.46032784325685	-1.67388803036527
C	-2.80140043196282	0.26339562529694	3.40892709485478
H	-3.33029612005162	0.34567965954575	4.36120401143300
N	6.70653499170688	0.02588837657633	-2.24471052294464
C	7.25273516415807	-0.09905734411960	-3.57956865783098
H	6.90974476521997	0.71471239680866	-4.23967486888564
H	8.34564892047996	-0.04974682800598	-3.52338420114728
H	6.98013770252540	-1.06054057201230	-4.04504515636167
C	7.60951029599017	0.18888382712164	-1.12739602983697
H	8.64135112330369	0.19469494684557	-1.49503987731897
H	7.43053740878868	1.13858020425838	-0.59563362830447
H	7.50971891117880	-0.63477578246535	-0.40053861342492
H	-0.86184030527276	-0.28997357698149	-2.20697167395748

[2-dimethylamino-pBiphe-H]⁺ (**23**), S_{0,eq} in methanol

N	1.22742892369049	-0.12168260215152	-1.50524741078341
C	1.43461581150340	0.16150852358062	0.89476865594821
C	0.68478649455812	-0.00880836180051	-0.30973607758829
C	3.44942325590652	0.08383196436883	-0.51959715367407
C	0.77625694963816	0.27911032564426	2.14926843470554
C	2.84845194897471	0.20967664242585	0.79603736631760
C	2.56082874979001	-0.07991834441683	-1.63622928544162
C	3.59772584006235	0.37811265293692	1.97586312540123
H	4.68708799674663	0.41811990873461	1.93758090745738
C	4.82480484715560	0.11636242109076	-0.74079478515684
H	5.49386165664644	0.23986017939269	0.10753279753038
C	1.56238136767320	0.44841429267606	3.28726167720382
H	1.10184645026397	0.54792963146821	4.27064329695766
C	4.46971145534496	-0.16643783227651	-3.14068318308696
H	4.85674209658672	-0.26221932974229	-4.15452820222249
C	3.11977870242688	-0.20149129058626	-2.93770717425231
H	2.43281603049628	-0.32402024975919	-3.77799712558551
C	5.37276997581261	-0.00618611757581	-2.03695330257265
C	2.95810467099570	0.49581854726173	3.19684124663207
H	3.54765965513893	0.62814112353352	4.10679750923837
N	-1.43735857651784	-0.21799479242038	-1.36139254233716
C	-1.44085582638790	0.05391003971780	1.00372247274023
C	-0.75540057693610	-0.05998486074369	-0.23565668548337
C	-3.56438531329275	-0.17625705694492	-0.25344555651307
C	-0.69133413848546	0.22006325321867	2.20505553064985
C	-2.86405246429567	-0.00442259268032	1.00882780528182
C	-2.80608691303758	-0.28275350827138	-1.44271832326832
C	-3.52753496585095	0.10526156167128	2.23990231815388
H	-4.61579933441875	0.06786143165333	2.28936957897487
C	-4.96675062702687	-0.24474719708850	-0.36947997526307
H	-5.59023278462578	-0.16840402785733	0.52195986214150

C	-1.40305227119593	0.31823805844276	3.39912604116071
H	-0.88062775300599	0.44008130609404	4.34812078550962
C	-4.79577909851354	-0.51331185965486	-2.76990779213923
H	-5.28069692246164	-0.64365206296227	-3.74008250237125
C	-3.41783131771148	-0.45156306728432	-2.69473334056466
H	-2.79252712880110	-0.53048617958944	-3.58699011371697
C	-5.57126739301359	-0.40925013618474	-1.60311454271291
H	-6.66045505226340	-0.45872808548597	-1.66825747768662
C	-2.79910040857359	0.26179049587945	3.40855431346985
H	-3.32699120161422	0.34318593593533	4.36166002225201
N	6.70855366981756	0.02578579196177	-2.24212311566369
C	7.25640006210578	-0.09855370651960	-3.57659127372300
H	6.91435024761818	0.71572515378565	-4.23660588208665
H	8.34933030094706	-0.04969690332026	-3.51868859051627
H	6.98376975051394	-1.05954500347266	-4.04311528945005
C	7.61011120652904	0.18806064266889	-1.12311667676465
H	8.64240810417928	0.19448706939834	-1.48969975597674
H	7.42994445364873	1.13703712150137	-0.59049285523164
H	7.50935074219736	-0.63602509869314	-0.39689697766183
H	-0.87278134893862	-0.29133380756004	-2.21421077823126

[2-dimethylamino-pBiphe-H]⁺ (**23**), S_{0,eq} in dimethyl sulfoxide

N	1.22781167622338	-0.12173668044485	-1.50397273259046
C	1.43507645275272	0.16154273394306	0.89585728336676
C	0.68529640181290	-0.00885575132569	-0.30882843631062
C	3.44976896118074	0.08382116824265	-0.51876795185740
C	0.77643685701971	0.27915869916171	2.15014585591811
C	2.84886656481022	0.20972412885608	0.79697939774720
C	2.56080453087519	-0.08003315788299	-1.63546239198822
C	3.59806589581974	0.37825518747437	1.97681013734222
H	4.68735140304117	0.41826032343245	1.93809527907784
C	4.82496316192339	0.11634852212585	-0.74046956872500
H	5.49439517025112	0.23985580856119	0.10754886529379

C	1.56250617151403	0.44854908474431	3.28815709118016
H	1.10159315576898	0.54806798843732	4.27128975139357
C	4.46879752167188	-0.16663808097603	-3.14081594871520
H	4.85600063598434	-0.26241287427533	-4.15450399274121
C	3.11897620155469	-0.20171574986759	-2.93738737078942
H	2.43060319014214	-0.32423029625096	-3.77644034459838
C	5.37235400231169	-0.00625803278721	-2.03715857921494
C	2.95825678455921	0.49599245525297	3.19773318961869
H	3.54764840897028	0.62837767093125	4.10762741969804
N	-1.43619995366242	-0.21803268398527	-1.36097119481168
C	-1.44066881309991	0.05392701451240	1.00424394856047
C	-0.75510999520931	-0.06003579728623	-0.23514426673588
C	-3.56344437397792	-0.17619809803054	-0.25386908077467
C	-0.69125521953261	0.22005676287991	2.20561795356103
C	-2.86375448243269	-0.00441296852261	1.00880021530819
C	-2.80452818058298	-0.28276572563245	-1.44304057802418
C	-3.52758747612735	0.10519383369894	2.23969956908638
H	-4.61581241163851	0.06771628650964	2.28844180567670
C	-4.96570554767606	-0.24457143348228	-0.37045871954396
H	-5.58912013449231	-0.16812128046095	0.52093478744010
C	-1.40328742516389	0.31814835998753	3.39948194255551
H	-0.88080498566525	0.43993159081621	4.34837990802838
C	-4.79379328090482	-0.51320249211963	-2.77087392795230
H	-5.27839051389938	-0.64350942804555	-3.74106459162439
C	-3.41587674174714	-0.45158157588685	-2.69536143875801
H	-2.78984985280611	-0.53051906916336	-3.58697453623993
C	-5.56968934869883	-0.40904123496894	-1.60435661532560
H	-6.65872198774083	-0.45841710429463	-1.66994487861856
C	-2.79937137075301	0.26166041807100	3.40850428698185
H	-3.32737418214644	0.34297730465194	4.36140066010760
N	6.70745454781533	0.02579933026453	-2.24275351516948
C	7.25459666098661	-0.09862856954297	-3.57689930272057
H	6.91099648251188	0.71523651112192	-4.23653936578827

H	8.34741282065725	-0.04970591110961	-3.51883687881891
H	6.98045716580257	-1.05933099576972	-4.04300889573161
C	7.60907602261984	0.18810527057623	-1.12450419257602
H	8.64094897502022	0.19455101527213	-1.49196792965682
H	7.42762330835106	1.13666869008947	-0.59168021749649
H	7.50722005144764	-0.63568656744000	-0.39817936429660
H	-0.87061290544227	-0.29138460006280	-2.21341253974776

[2-dimethylamino-pBiphe-H]⁺ (**23**), S_{0,eq} in water

N	1.22716958891036	-0.12325606098804	-1.51113363144209
C	1.43354075067919	0.16053332959696	0.88950484656173
C	0.68384966232784	-0.00992934808320	-0.31499230281435
C	3.44871058707243	0.08303441709112	-0.52291500413101
C	0.77640190428565	0.27839917391703	2.14447381655102
C	2.84714889382226	0.20859168531013	0.79187189194340
C	2.56160981086267	-0.08117705739319	-1.64010696477222
C	3.59696925732169	0.37648956054942	1.97132070453721
H	4.68602581235201	0.41557975075677	1.93144263807817
C	4.82449531401785	0.11654890208319	-0.74098032668457
H	5.49194643066688	0.24096074455903	0.10843324307952
C	1.56233030041539	0.44749546834369	3.28248959537264
H	1.10070370402167	0.54696515614392	4.26506995099385
C	4.47401628927148	-0.16710944033856	-3.14065692546873
H	4.86396775007008	-0.26292513503615	-4.15315923598867
C	3.12373610664634	-0.20278011014088	-2.94017249751458
H	2.44058591896078	-0.32591450527601	-3.78281074497739
C	5.37446061615864	-0.00600833822897	-2.03563279763342
C	2.95799392023476	0.49439387778891	3.19248606885387
H	3.54740784126442	0.62628430759760	4.10207678283031
N	-1.44113815184099	-0.21900748533005	-1.36358770400583
C	-1.44046583388741	0.05362482513393	1.00086985175215
C	-0.75611167552564	-0.06075899005258	-0.23919442456644
C	-3.56634952362190	-0.17580678846424	-0.25173468102063

C	-0.69056301287104	0.21977397142845	2.20157690104398
C	-2.86357067744148	-0.00419956968604	1.00867491321086
C	-2.81048934099948	-0.28309152374862	-1.44162967622080
C	-3.52577132333799	0.10559397383539	2.24030533229542
H	-4.61378674958985	0.06803227330636	2.28962513620899
C	-4.96891878428543	-0.24322281738993	-0.36483463238057
H	-5.58964108154995	-0.16580739015171	0.52812173777607
C	-1.40038339626928	0.31836111603986	3.39664781196333
H	-0.87574015504193	0.44028893364695	4.34411920036513
C	-4.80209386507652	-0.51295808329756	-2.76536357237192
H	-5.28849345239080	-0.64336873988298	-3.73430378313559
C	-3.42405301201338	-0.45203641475687	-2.69237812774405
H	-2.79923089815754	-0.53154325973016	-3.58451815094306
C	-5.57563634864443	-0.40780686737909	-1.59730327921388
H	-6.66454085385459	-0.45646871842839	-1.66063874165471
C	-2.79631022119161	0.26215988185836	3.40822787015403
H	-3.32272187216017	0.34370014865277	4.36164302616632
N	6.71101849376955	0.02671887737930	-2.23846442001633
C	7.26141084145898	-0.09738737499881	-3.57273103901522
H	6.91947262946189	0.71604119186819	-4.23289114778651
H	8.35370005820756	-0.04760836289322	-3.51208283908921
H	6.98986589617928	-1.05805265538877	-4.03920020648016
C	7.61040136634653	0.19011664975471	-1.11689442020663
H	8.64276224578687	0.19707572114056	-1.48191923280022
H	7.42787783989116	1.13849595130899	-0.58520204049436
H	7.50814402447243	-0.63326224515183	-0.39096777272715
H	-0.88131362518536	-0.29287260687576	-2.21848099643768

[2-dimethylamino-pBiphe-Me]⁺ (**24**), S_{0,eq} in vacuum

N	1.29962393556384	-0.11134885547261	-1.52552664636286
C	1.45411564244291	0.31764916597450	0.84512404062459
C	0.70874920863369	0.13825855729876	-0.37001860003004
C	3.50299526414063	0.12646986738766	-0.51316046447855

C	0.79467958083944	0.42856756996398	2.09386892829953
C	2.87140343999584	0.35834497735925	0.77035928884753
C	2.63185267854202	-0.14353341702834	-1.61935835556435
C	3.60224228736425	0.59405476837412	1.94831396303665
H	4.69095279300472	0.64066159769405	1.91770690957303
C	4.88075944972541	0.12868072785476	-0.71465783269768
H	5.53732375085319	0.34124101217927	0.12483351681958
C	1.56207813821564	0.66673609228444	3.23359925381238
H	1.08674308958078	0.77820030521334	4.20786448931303
C	4.56270631272564	-0.43944477062951	-3.06764015282315
H	4.96574492400002	-0.66610675035509	-4.05326279913324
C	3.21051152410228	-0.43483332369288	-2.88655533618448
H	2.53269880734741	-0.65239737341784	-3.71371913597733
C	5.44861222820908	-0.14747699098081	-1.97742036250913
C	2.95300763376931	0.76238208092020	3.15755001905247
H	3.52983768866019	0.95342101521728	4.06441230201732
N	-1.47993063814368	0.24884952374776	-1.45996039113330
C	-1.40371222821310	0.08371494097352	0.93791505908102
C	-0.74316734523783	0.16260327887798	-0.33022544210514
C	-3.52446381601320	-0.30000147609601	-0.25807541593834
C	-0.65556654255108	0.24400025924678	2.14431987756093
C	-2.81300950721542	-0.10279552767732	0.98718329218225
C	-2.83403262794329	-0.10300727273258	-1.47429254850578
C	-3.45896458780338	-0.11010297449341	2.22986623549323
H	-4.53947085524672	-0.23404316112274	2.28806090500072
C	-4.88148648843350	-0.67138089668688	-0.31001189871114
H	-5.42665320494051	-0.84276958731168	0.61774329782588
C	-1.34808889256183	0.22247965713918	3.35420849374398
H	-0.80998425008002	0.33814809777036	4.29402339493317
C	-4.83931603174560	-0.64848884945578	-2.71392421230781
H	-5.34145497147705	-0.80072901966389	-3.67132765536954
C	-3.50590166999959	-0.28271582464026	-2.69830764070831
H	-2.97962995025378	-0.17185210634999	-3.64400197863205

C	-5.53588132463103	-0.84025929962484	-1.51453045584874
H	-6.58707457459422	-1.13341078015125	-1.52950129837448
C	-2.73009296447455	0.05115354908158	3.39583519049031
H	-3.24202042007145	0.04401136309703	4.36031592050389
N	6.78925955862508	-0.14403069820755	-2.16446552507131
C	7.35622124070993	-0.43557217321438	-3.46483131729127
H	7.02244047387951	0.28694119450593	-4.22742653059974
H	8.44791473536226	-0.37430052236027	-3.40167639429160
H	7.09508675143073	-1.45037689757123	-3.80723207718586
C	7.67477540900662	0.14699400390973	-1.05895025312241
H	8.71305344371411	0.10572175222574	-1.40487966084286
H	7.49354131310156	1.15453690536647	-0.64857865628128
H	7.55989907519644	-0.58584738318139	-0.24264991923459
C	-0.93577021718210	0.79758617542911	-2.70363799722388
H	-0.07405976306780	1.42749465313271	-2.47741385953457
H	-0.60974269815716	0.00816374593504	-3.39162603532445
H	-1.72035480870476	1.40865909395800	-3.16545752881219

[2-dimethylamino-pBiphe-Me]⁺ (**24**), S_{0,eq} in chloroform

N	1.29917627954224	-0.13425687095181	-1.51956394578591
C	1.45392773970375	0.31364650589894	0.84627652879976
C	0.70808132893615	0.12721469282849	-0.36750735013659
C	3.50367240360018	0.12002888322835	-0.51266223419359
C	0.79427931866251	0.42623454092757	2.09536109770999
C	2.87172750107185	0.35296931275882	0.77183642286739
C	2.63167156256171	-0.16202803434281	-1.61567335243192
C	3.60405641738716	0.58640415692132	1.94998209894904
H	4.69317809923668	0.63128665738100	1.92001075033744
C	4.88129137854648	0.13017374300630	-0.71483148156557
H	5.53934843116472	0.35202919167365	0.12164017013543
C	1.56166149714453	0.65807840232616	3.23696743031700
H	1.08629471354777	0.76286185891444	4.21223953750334
C	4.56205947196184	-0.45545260335825	-3.06636404309570

H	4.96588311131034	-0.68351307946864	-4.05186392931547
C	3.20962691109204	-0.45838896375959	-2.88234819387515
H	2.53301725647066	-0.68265741520874	-3.70963455474378
C	5.44819632971077	-0.15026025048221	-1.97881477661992
C	2.95315987091222	0.75145272856693	3.15958611083335
H	3.53058858224231	0.93745673682280	4.06762893956158
N	-1.47713392822075	0.24954557168560	-1.45852237402498
C	-1.40430390507928	0.07964603197208	0.93927222580749
C	-0.74366025726186	0.15769059097919	-0.32959993276523
C	-3.52223747136865	-0.30430392473693	-0.25895336522977
C	-0.65733841283711	0.24554834304585	2.14535523809011
C	-2.81295153238205	-0.10689097551919	0.98803575354891
C	-2.83072905113025	-0.10077470615340	-1.47390764238569
C	-3.46140797194024	-0.11028731562877	2.23025482097298
H	-4.54211802156677	-0.23594304455529	2.28816194064394
C	-4.87921292480233	-0.67784309039802	-0.31207695932563
H	-5.42505625057931	-0.85260739013645	0.61516514310391
C	-1.35070309070703	0.23426263521469	3.35554243807839
H	-0.81443633123221	0.36164337066777	4.29535537844274
C	-4.83438842451660	-0.64081997708808	-2.71755350944715
H	-5.33602063064298	-0.78669953414233	-3.67672949140554
C	-3.50144846810251	-0.27243528102568	-2.70016672133475
H	-2.97426995721612	-0.14994558670152	-3.64421163925983
C	-5.53128941301285	-0.84179914602431	-1.51923222804162
H	-6.58241584943250	-1.13689495604959	-1.53642177819490
C	-2.73298125266503	0.06074819162698	3.39555935167860
H	-3.24609183553680	0.06045585932589	4.35979289887919
N	6.78638470630115	-0.13779666078478	-2.16753277397273
C	7.35459520606718	-0.43840883046984	-3.46505010123143
H	7.01686977289457	0.27562368486514	-4.23411500471827
H	8.44613372100660	-0.37328640828887	-3.40033115544581
H	7.09432496991623	-1.45613885350091	-3.79934508088722
C	7.67203722761465	0.17077244502731	-1.06669228117828

H	8.70874471091013	0.14329277297866	-1.41913637503166
H	7.47616362471044	1.17641280111008	-0.65862412090358
H	7.56988628392871	-0.55882313151777	-0.24577861412796
C	-0.93252634450230	0.80476453879080	-2.69956938883141
H	-0.06619708123233	1.42772311169912	-2.47101161082063
H	-0.62641092294861	0.01872480799122	-3.40048559097031
H	-1.71170909923926	1.43046386205865	-3.15091267496256

[2-dimethylamino-pBiphe-Me]⁺ (**24**), S_{0,eq} in methanol

N	1.29830489994480	-0.14749019628590	-1.51927281399790
C	1.45348259278201	0.31286458204572	0.84431952062782
C	0.70764370935049	0.12193167855598	-0.36850848235981
C	3.50303932562822	0.11751668293408	-0.51394984531318
C	0.79405817901308	0.42644087176932	2.09357192977422
C	2.87113079723967	0.35369805977264	0.76989484678242
C	2.63135872094272	-0.17322368385902	-1.61496138727523
C	3.60378347381899	0.59088056924502	1.94715699745706
H	4.69306226268423	0.63740148670579	1.91765360564089
C	4.88058054113770	0.13139528269901	-0.71554971073883
H	5.53813554529391	0.36008306618248	0.11976632876466
C	1.56097986821344	0.66118222986514	3.23487437292055
H	1.08596577624591	0.76596554872952	4.21052846684617
C	4.56305228157939	-0.46844693807587	-3.06414187555420
H	4.96707048920070	-0.69990228606060	-4.04902225654465
C	3.21058100095330	-0.47500152320443	-2.87978299697148
H	2.53615333989344	-0.70519559541927	-3.70754073939212
C	5.44811423667548	-0.15394527482752	-1.97838213349372
C	2.95236325973466	0.75708354818887	3.15648354761652
H	3.52981706939267	0.94567681065350	4.06422621709276
N	-1.47687787236775	0.25157441116388	-1.45755025647088
C	-1.40381231812514	0.07547203818544	0.93910579802043
C	-0.74351002529444	0.15505567378659	-0.32970673385457
C	-3.52119297975735	-0.30701061556565	-0.25922566053375

C	-0.65697921771942	0.24263585153327	2.14468744659810
C	-2.81198058044822	-0.11211683621426	0.98798797018308
C	-2.83030848552041	-0.09810586365621	-1.47347472212179
C	-3.46036952030693	-0.11751084502117	2.23030570080731
H	-4.54113383251351	-0.24424534382473	2.28915610242205
C	-4.87792595995580	-0.68142616825065	-0.31291148824369
H	-5.42405430431733	-0.86031492539666	0.61367381661362
C	-1.34942419764127	0.23031319241116	3.35542941670585
H	-0.81362147479975	0.35934083207297	4.29556152718360
C	-4.83325604602985	-0.63328860241033	-2.71880522186557
H	-5.33513398047278	-0.77483122899157	-3.67875466229219
C	-3.50059554457715	-0.26391475814686	-2.70054743921639
H	-2.97387224505362	-0.13578563327493	-3.64435800018617
C	-5.52966811024382	-0.84055119524593	-1.52106820004835
H	-6.58081095053821	-1.13640924862430	-1.53935621655219
C	-2.73148684189275	0.05410000688607	3.39534911258693
H	-3.24438648078175	0.05269695112833	4.35989326865874
N	6.78554161559851	-0.13736643281178	-2.16718951916422
C	7.35482518296247	-0.44514958881549	-3.46280743907560
H	7.01652145178222	0.26381905877455	-4.23633437201003
H	8.44631625647480	-0.37851772709200	-3.39763754218886
H	7.09559479981441	-1.46510035931104	-3.79094110640301
C	7.67011521756251	0.18226140215248	-1.06816045313828
H	8.70663415443880	0.15997755940142	-1.42173193643187
H	7.46778063067222	1.18840735296462	-0.66471865387183
H	7.57335068177494	-0.54392817434240	-0.24361284943218
C	-0.93368279879655	0.81662001204019	-2.69507359818800
H	-0.06497538786059	1.43491222638776	-2.46232317515105
H	-0.63602305572453	0.03707101942877	-3.40666435994752
H	-1.71127515006691	1.45130103906396	-3.13676014527365

[2-dimethylamino-pBiphe-Me]⁺ (**24**), S_{0,eq} in dimethyl sulfoxide

N	1.29916137097344	-0.14344448858325	-1.51859156973320
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C	1.45396061241306	0.31147406366498	0.84570337708543
C	0.70809520907071	0.12241487073917	-0.36759607609589
C	3.50373912466505	0.11739729927528	-0.51286439090703
C	0.79437088671526	0.42472510302024	2.09475245120553
C	2.87166434393440	0.35098629003817	0.77146995391164
C	2.63172063952743	-0.16950638739419	-1.61479532864605
C	3.60445145936010	0.58472756945298	1.94925645820786
H	4.69372565704989	0.62965955946026	1.91958554311180
C	4.88113365207482	0.13075141895309	-0.71454099362850
H	5.53913676625278	0.35673275755379	0.12113818385756
C	1.56142519545737	0.65603295971152	3.23668874352928
H	1.08609709732104	0.75981230920449	4.21221667357701
C	4.56252507152367	-0.46211270847866	-3.06538425210275
H	4.96670814129639	-0.69115050658712	-4.05066384188672
C	3.21012452430270	-0.46800402285377	-2.88083761092415
H	2.53445601985950	-0.69518503496050	-3.70832503234691
C	5.44814626096025	-0.15146011859838	-1.97863330621318
C	2.95296672860362	0.74940133985738	3.15877326586768
H	3.53047326722619	0.93503618555565	4.06694249358664
N	-1.47586893522958	0.24858798857872	-1.45823643383825
C	-1.40391653750515	0.07761453532631	0.93923369027224
C	-0.74343370615461	0.15504778940802	-0.32986569823488
C	-3.52116457478882	-0.30447354655707	-0.25909254879047
C	-0.65717739745458	0.24451181966100	2.14493808985968
C	-2.81223828856476	-0.10818760469887	0.98803448675902
C	-2.82932654286024	-0.09987873479602	-1.47367748781825
C	-3.46117675611779	-0.11096010992212	2.23007399190373
H	-4.54203202512594	-0.23640522157231	2.28836424483241
C	-4.87845955927038	-0.67679305059416	-0.31208962568834
H	-5.42479967022672	-0.85183913407282	0.61498976165277
C	-1.35013740639148	0.23513481567016	3.35538164087547
H	-0.81422363273916	0.36468690709731	4.29527725100772
C	-4.83296475613204	-0.63599791074351	-2.71795775171121

H	-5.33467157536922	-0.77961156279573	-3.67754196382496
C	-3.49978712206654	-0.26862058033947	-2.70048390622816
H	-2.97246363034638	-0.14413295185563	-3.64431062787439
C	-5.53009969328428	-0.83844183928492	-1.51990297998291
H	-6.58159976729118	-1.13258869689418	-1.53760324620363
C	-2.73248184885861	0.06139975105111	3.39505443872409
H	-3.24566791499890	0.06235820352597	4.35930404312428
N	6.78497716841565	-0.13543719840065	-2.16756142447498
C	7.35345229149852	-0.43767395726463	-3.46429058134049
H	7.01212842371836	0.27332036992411	-4.23454126118131
H	8.44474598272154	-0.36962995500102	-3.39925813584624
H	7.09383084591773	-1.45640038839106	-3.79580110220683
C	7.66974996051162	0.17942842800159	-1.06797330294007
H	8.70606418541257	0.15469987251851	-1.42162854660111
H	7.46862770108006	1.18489138450618	-0.66226170116831
H	7.56897374760039	-0.54788957071959	-0.24499481476005
C	-0.93099512492039	0.80503847726673	-2.69863275356336
H	-0.06281675946604	1.42504691681702	-2.46895775394299
H	-0.63121278671376	0.01936627660443	-3.40262054389469
H	-1.70891632358768	1.43444001891544	-3.14686218835152

[2-dimethylamino-pBiphe-Me]⁺ (**24**), S_{0,eq} in water

N	1.29765104791787	-0.18620064017836	-1.51649740539098
C	1.45332979995164	0.27599513287850	0.84745223470869
C	0.70776076643104	0.09124365399668	-0.36634060451692
C	3.50265887565375	0.07207490276355	-0.50795484718362
C	0.79439930388361	0.38798699558490	2.09705212904732
C	2.87084177110072	0.31073194824955	0.77492445804519
C	2.63182941409119	-0.21886424103831	-1.60922768352155
C	3.60409583445988	0.54295433978125	1.95276031702846
H	4.69329318759042	0.58458669860462	1.92273379073170
C	4.88064626704256	0.08246777965585	-0.70628539811145
H	5.53679768877865	0.31208416755919	0.12981468260728

C	1.56122049358601	0.61733165564108	3.23932664747880
H	1.08491490571174	0.72043223272486	4.21425789811860
C	4.56657014702814	-0.52452239690678	-3.05265623594675
H	4.97287857994517	-0.75992328311644	-4.03543737381547
C	3.21364605535178	-0.52698042093441	-2.87125215886996
H	2.54273739663519	-0.75805422431678	-3.70094018180388
C	5.44965286802558	-0.20788216961164	-1.96666333254714
C	2.95291947538237	0.70925265683799	3.16211210183834
H	3.53034621945285	0.89387115126458	4.07017691101198
N	-1.47722109852406	0.25151306261842	-1.45220801104321
C	-1.40402423138359	0.05214819237284	0.94169465548321
C	-0.74308457786774	0.13712024443538	-0.32626658457543
C	-3.52528554105987	-0.30271019033007	-0.25838129956150
C	-0.65656110783623	0.20709668162467	2.14809325156299
C	-2.81311464654750	-0.12806902443887	0.98989681855587
C	-2.83473579171251	-0.08334190129736	-1.47044874102295
C	-3.46048586121076	-0.14355127008821	2.23267198678816
H	-4.54146799631836	-0.26662192821025	2.29086680736800
C	-4.88526944770043	-0.66431401019117	-0.31494349245738
H	-5.43103573607788	-0.85072532034554	0.61003372987118
C	-1.34771594542816	0.18675192129065	3.35931487873417
H	-0.80994757761227	0.30644088779268	4.29929833001324
C	-4.84388856070233	-0.58104253972520	-2.72009607953980
H	-5.34863530528700	-0.70325074301493	-3.68070841923333
C	-3.50796026160079	-0.22397973941598	-2.69873277361668
H	-2.98105752212591	-0.08537471284270	-3.64071313194124
C	-5.54003592804900	-0.80023761847367	-1.52427224095303
H	-6.59338563392618	-1.08636911393450	-1.54515138663735
C	-2.73020124661500	0.01406598388091	3.39881134103748
H	-3.24227181974410	0.00510391550311	4.36327051319955
N	6.78789031532603	-0.19396346480643	-2.15315187258304
C	7.35937956065946	-0.51466812499176	-3.44552721625690
H	7.02670283299116	0.18971531456939	-4.22487505138459

H	8.45049773178257	-0.45317642744665	-3.37686978503060
H	7.09507167229483	-1.53506352275653	-3.76626478197005
C	7.67081992066536	0.12733250649649	-1.05225955427365
H	8.70704153595261	0.10824504847134	-1.40560933514935
H	7.46473794909158	1.13201819948233	-0.64881265912511
H	7.57483314034474	-0.59908882176247	-0.22846978575802
C	-0.93141676257797	0.82908237331991	-2.68299219893183
H	-0.05037994564646	1.42600314204044	-2.44421502344420
H	-0.65685840692744	0.05818944190518	-3.41215609434072
H	-1.69984471864701	1.48643123182868	-3.10637535869249

10-dimethylamino-pBiphe (**25**), S_{0,eq} in vacuum

N	1.37645065386408	0.14672212902839	-1.33229380743541
C	1.47256994709553	-0.09110001860528	1.07201941307767
C	0.77267225348586	0.03342483738903	-0.18593552390220
C	3.55298596656018	-0.04269342924990	-0.22735903857151
C	0.74070970903047	-0.28583451445694	2.27631750540846
C	2.89457136338904	-0.00933804133462	1.06641754834180
C	2.72996526034023	0.06540395909598	-1.38614399186425
C	3.57634108243566	0.05228100258477	2.32682996348005
C	4.93810250024661	-0.25463975440739	-0.43074940985055
H	5.57576938638106	-0.40878856663769	0.43740097213067
C	1.46354138938274	-0.38101787479201	3.45888921455783
H	0.95248447883417	-0.54631697519668	4.40746547970335
C	4.66860007759794	-0.12304633281741	-2.83651027366848
H	5.10972029582408	-0.14289252024445	-3.83576492879485
C	3.31270792648915	0.05200040356009	-2.67582293445175
H	2.63168335623620	0.16039309273027	-3.52161559466259
C	5.47907504864369	-0.30131473403396	-1.70072818080254
H	6.55026307442497	-0.48160722606672	-1.81958077046161
C	2.84251456410689	-0.19327843752482	3.48574139358156
H	3.34674640069453	-0.18885699363651	4.45184764163534
N	-1.30414476903968	0.25329798709273	-1.33907866591964

C	-1.42530301917359	-0.18438526321960	1.03212426034020
C	-0.71134617076189	0.04812558308186	-0.19762397665728
C	-3.49380880343253	0.00704563224375	-0.27840366487933
C	-0.72552423802797	-0.37844763491468	2.25419650590407
C	-2.84362999355435	-0.22283347002790	0.99198226659946
C	-2.66231674303285	0.24745985661988	-1.40655247740281
C	-3.55110209317383	-0.48116055517192	2.18195389471867
H	-4.64052058474569	-0.52045678619818	2.17529660724178
C	-4.89276294659296	0.01075187328461	-0.45845090453574
H	-5.55219660526887	-0.17153287014452	0.39152172113474
C	-1.47032625769697	-0.63872528451153	3.40237071874367
H	-0.97159490762578	-0.80837865125593	4.35653617840280
C	-4.62323397534388	0.48644230940210	-2.81686062929645
H	-5.07151461051382	0.67145110389677	-3.79581102502905
C	-3.25323011563746	0.48624289298285	-2.66991728855360
H	-2.57649995976826	0.66534412321484	-3.50716908002252
C	-5.44787677535802	0.24586171609602	-1.70142870109796
H	-6.53411349933540	0.24522873567171	-1.81803732289439
C	-2.86721876063473	-0.69109850211150	3.36327533786365
H	-3.42079142390493	-0.89821391563605	4.28203217482774
N	4.93779534144906	0.36597312041299	2.40483278011021
C	5.32570102932091	1.67164726649071	1.90716002868210
H	5.16077845298843	2.45894270221645	2.66973899968856
H	6.39265536797045	1.67345345633273	1.63361893608671
H	4.74949064178844	1.93654488704609	1.01311687852867
C	5.65655166286689	-0.01282798037161	3.59282306813369
H	6.73665802616909	0.06734784489622	3.39614382132496
H	5.43373160444577	0.62784929129634	4.47198089321133
H	5.43611939056127	-1.05624947409941	3.85810398729476

[10-dimethylamino-pBiphe-H]⁺ (**26**), S_{0,eq} in vacuum

N	1.33957763638546	0.19484127359997	-1.28777766244119
C	1.46484183380017	-0.09087373361886	1.12251175905051

C	0.77040155813228	0.04986860198467	-0.11887830306701
C	3.51361878786345	-0.03560528243072	-0.20933151262859
C	0.73604519335390	-0.32078658680203	2.31831548561706
C	2.88303057520006	-0.00291870553103	1.09068363527979
C	2.68561349602303	0.11245407756964	-1.37239006098458
C	3.58386021467782	0.03169719835939	2.35148337035392
C	4.88937213623503	-0.28614127615028	-0.42803703371971
H	5.53021889767571	-0.48933518719416	0.42765092677784
C	1.48423001505380	-0.49871934322936	3.48209301329450
H	0.98941027025486	-0.72051353500863	4.42827234146331
C	4.60989813121518	-0.07533215639576	-2.83273867755800
H	5.05116111112409	-0.07890751398429	-3.83131949871153
C	3.26167858682455	0.12666657154991	-2.66748098611555
H	2.59052493506495	0.26963243453495	-3.51583010680065
C	5.41781571786128	-0.31520786085295	-1.70167834407726
H	6.48000771091742	-0.53245980370283	-1.83458710589246
C	2.86199092269687	-0.32553968598809	3.50041289296096
H	3.37597409502460	-0.38874660805998	4.45847154380994
N	-1.29802946797737	0.21286960518529	-1.27467088585699
C	-1.42398034202746	-0.17489951877430	1.06876714638423
C	-0.68453620569045	0.03695994921269	-0.11293824551598
C	-3.47992867772400	0.01073195409959	-0.30187916861137
C	-0.72293603186086	-0.37360505447479	2.29775347424559
C	-2.84993672214724	-0.19890170144103	0.99060128228490
C	-2.66214597918284	0.21608432457572	-1.43994544761677
C	-3.56817641900100	-0.42975056633890	2.16919906922745
H	-4.65715619629455	-0.45855942534796	2.16083143516192
C	-4.87452549667879	0.01946684193623	-0.49942839047774
H	-5.54158922571766	-0.13310490752150	0.34899259881615
C	-1.49685011294842	-0.60413945985683	3.43584403202899
H	-1.02182783265576	-0.76585102635550	4.40310736535322
C	-4.58375278239862	0.41983380984764	-2.86843483667999
H	-5.01992053217336	0.57704899633987	-3.85677178201663

C	-3.21141368663655	0.41864420457843	-2.71545991040597
H	-2.54947888751512	0.57338457922203	-3.57051390347975
C	-5.41688084487886	0.21991005354915	-1.75515096654877
H	-6.50103153722691	0.22276031712642	-1.88206200129192
C	-2.89043142542907	-0.62930665801075	3.36478060253263
H	-3.46270186786123	-0.81042120744314	4.27733035889952
N	4.90478368964012	0.40253549320537	2.44002574153710
C	5.34932995209553	1.63208739639481	1.80587882869092
H	5.41424343520071	2.43909100816013	2.55779637176105
H	6.34263276611280	1.50701065587931	1.34799179406734
H	4.64955296381604	1.95109512114102	1.02669386391611
C	5.65727060507817	0.06551065996750	3.62633873542663
H	6.72832147661532	0.17976484377789	3.40747042367562
H	5.41905693135087	0.71900593829268	4.48747856751037
H	5.48120689049037	-0.98000095162579	3.91247151185992
H	-0.66014026175837	0.34187184604915	-2.06744334148911

[10-dimethylamino-pBiphe-Me]⁺ (**27**), S_{0,eq} in vacuum

N	1.40528907109307	-0.01025199600911	-1.32487917963802
C	1.47387301759300	-0.04869616488513	1.08982597617271
C	0.78985051874227	0.05394191165635	-0.17020601991249
C	3.55175752473986	-0.20444509059574	-0.18585257138703
C	0.74311126404936	-0.24561637764597	2.28296980168267
C	2.89500756477619	0.00979201619934	1.07995813820585
C	2.73909127598374	-0.20732597196084	-1.36542852329549
C	3.57526245531725	0.15876092382008	2.34290435624478
C	4.92188783020960	-0.52316903793036	-0.34304994857251
H	5.55129751014139	-0.60643122444553	0.54076613685472
C	1.47012850859169	-0.32432772025864	3.47346353329514
H	0.96038031070965	-0.49789597010302	4.42143966242058
C	4.66171650693785	-0.71300149924672	-2.75282418016236
H	5.10785958204907	-0.90210566355639	-3.73110979992341
C	3.32150029484272	-0.43702601595039	-2.63848958443343

H	2.65991406889551	-0.41199229114865	-3.50579714644332
C	5.45568709307550	-0.78025558672822	-1.58864659974553
H	6.51130982608840	-1.04868774227622	-1.67164074441357
C	2.83913569799662	-0.10818637145486	3.50820009038058
H	3.33519003049901	-0.08264762012178	4.47733580859047
N	-1.33118484490107	0.57003549845806	-1.28589355414625
C	-1.39598808607015	-0.21451462151736	0.98420671177226
C	-0.67374422893315	0.16382515689935	-0.18187370193585
C	-3.46274978463216	-0.15079705506525	-0.35546321948554
C	-0.69915654543872	-0.41525314243905	2.21948118067700
C	-2.81465779360136	-0.34566925714979	0.92315966769345
C	-2.69951464348197	0.32628735355388	-1.44542748801807
C	-3.51909005964031	-0.67607625437854	2.08489717865238
H	-4.60372559602318	-0.77094797627224	2.06662188861855
C	-4.83287752740756	-0.40643303627307	-0.55937964747560
H	-5.43548007327772	-0.78640765203742	0.26495459912275
C	-1.45433247001337	-0.75291225262033	3.34444059457414
H	-0.96229614372886	-0.92303553182996	4.30122837960690
C	-4.66018642093426	0.26694854633439	-2.86168868481905
H	-5.11801549940447	0.41345392807214	-3.84189932219702
C	-3.31343611834705	0.52955364887888	-2.69650493072834
H	-2.73380492022885	0.86100651040396	-3.55523624366141
C	-5.42876224720486	-0.19926165789222	-1.78720302032898
H	-6.49145685811597	-0.40875124821550	-1.92157780730656
C	-2.83869312930106	-0.87938981134124	3.27629100278665
H	-3.39718751439546	-1.14017319570035	4.17781748171090
N	4.88996838983828	0.54487824780545	2.41549096368281
C	5.36304164481888	1.67405585116914	1.63434561922503
H	5.46433743080110	2.56090386701206	2.28500656892807
H	6.34466880927382	1.46583628806034	1.18099819891033
H	4.65988451750726	1.91995096735707	0.83203214403219
C	5.62727443141342	0.33992481214102	3.64108333512868
H	6.70073972848711	0.43746408733515	3.42666906693179

H	5.37169073012103	1.07905644829462	4.42408969170467
H	5.45283983737332	-0.67051442518421	4.03414061723058
C	-0.67992898872762	1.36447262955933	-2.33077524235913
H	0.21590266822713	1.83796935816815	-1.92727549650994
H	-0.38445935908523	0.74519844031914	-3.18622297775594
H	-1.38796928729876	2.14038297073619	-2.64467276018179

2-trifluoromethyl-pBiphe (**28**), S_{0,eq} in vacuum

N	1.35982403961953	0.05091037259216	-1.38665256388603
C	1.45024921671694	-0.03513240104002	1.02603462851753
C	0.75288417026319	-0.00209296036624	-0.23604503771979
C	3.53527639823526	0.05043554732823	-0.27298341749262
C	0.74172214924941	-0.09274066402497	2.25797094956694
C	2.86932216625401	-0.00834135454032	1.00845733904223
C	2.71805408225437	0.07773956726375	-1.43639184664318
C	3.56590721003165	-0.03968354282115	2.23258338144290
C	4.93619866433647	0.08202866397737	-0.43323620768717
H	5.58685949619752	0.06210751642200	0.44228090165555
C	1.47562419076686	-0.12185189562170	3.44003585719463
H	0.96797503572666	-0.16585041529387	4.40343977147817
C	4.69367655220193	0.16551570003162	-2.84156631361220
H	5.15389325092573	0.21020308332626	-3.83125248048124
C	3.32225528457715	0.13555405023139	-2.71447127235785
H	2.65534085630620	0.15484111059179	-3.57803960487144
C	5.50466819373906	0.13841367016765	-1.69099910674389
H	6.59213357967468	0.16216649125918	-1.79212060593183
C	2.87420773141232	-0.09552700165323	3.42568535052840
H	3.42061224854871	-0.11952100754702	4.37112085836093
N	-1.33118963651465	0.00262124225383	-1.39696319807578
C	-1.43357709435321	-0.08706438392586	1.01645433818478
C	-0.72971535506550	-0.02867858405054	-0.24174628534496
C	-3.50939838008552	-0.07592293742637	-0.29511155537413
C	-0.73070394873146	-0.11941871482213	2.25287680904994

C	-2.85258125302394	-0.11133048022510	0.99149004077039
C	-2.68823349606247	-0.01950088185405	-1.45225549550431
C	-3.55718354664045	-0.16817069811555	2.20937540735718
H	-4.64715172364196	-0.18759405611943	2.21305777844832
C	-4.90886701428808	-0.09428514489918	-0.45902454483851
H	-5.56754605669685	-0.13773830789185	0.40783937535758
C	-1.47214680951004	-0.17565296191754	3.42950763679137
H	-0.96971376851115	-0.20201322375465	4.39623833140470
C	-4.65772974609641	-0.00346477286109	-2.87013632680575
H	-5.11814269124234	0.02295320585890	-3.85997367345121
C	-3.29015612548851	0.01583774302322	-2.73367490305141
H	-2.62231636892254	0.05814663722455	-3.59534406753463
C	-5.47139027650906	-0.05865507104195	-1.71879149155483
C	-2.87050978875553	-0.19972729642670	3.40638705004898
H	-3.42152823382655	-0.24395365405717	4.34838474074706
C	-6.96314576151699	-0.07158974046681	-1.89491467723039
F	-7.39030043923845	1.03954539570874	-2.50559645379499
F	-7.61130263781777	-0.16124806004418	-0.73043433924920
F	-7.35458861050614	-1.10261543332349	-2.65198354110165
H	4.65580621200792	-0.01987188112843	2.24302436939140

10-trifluoromethyl-pBiphe (**29**), $S_{0,eq}$ in vacuum

N	1.34778498503375	0.16651435852809	-1.40489321499306
C	1.48684709178449	0.04858300784052	1.00376623349611
C	0.76375853613463	0.08342812533671	-0.24780016403070
C	3.54578984569659	0.01792421898516	-0.33242510793682
C	0.76560744901867	-0.02011750164709	2.22912496961866
C	2.91429211583730	0.12768975691847	0.97404532171632
C	2.70074438154886	0.10274136892113	-1.47788207786487
C	3.58094452889002	0.32444873798913	2.22136416888628
C	4.91779658516434	-0.22881899934040	-0.56439165636610
H	5.59445054175549	-0.41570327591049	0.26176527462292
C	1.48178189942670	0.05493684188161	3.41581730970382

H	0.97586548556996	0.01108524870244	4.37913417407676
C	4.60571202201561	-0.11144204411331	-2.96568790790264
H	5.02665250791190	-0.14833121060018	-3.97299697608614
C	3.25455008724897	0.07105025758166	-2.77912849991533
H	2.55435479050585	0.16571455108480	-3.61056952966821
C	5.43375799360966	-0.28988816589842	-1.84453293063227
H	6.49904054532546	-0.49028227510979	-1.97931787905593
C	2.85623103087805	0.26299529899888	3.40201555859275
H	3.37373982176214	0.41304104651309	4.34898590618019
N	-1.32895722083404	0.13391512078500	-1.39171003903824
C	-1.41622097445845	-0.08836787586054	1.00762871488895
C	-0.71957454809320	0.05289681575462	-0.24407651221086
C	-3.50147278347816	-0.07511173478323	-0.28891166779734
C	-0.70113604796358	-0.14952136705771	2.23211712749636
C	-2.83230990306417	-0.17054882259827	0.98809458094658
C	-2.68681400189282	0.08435220799378	-1.44375900302819
C	-3.51813429478317	-0.34023066112151	2.20678262627369
H	-4.60601788894387	-0.41092415090957	2.21757183563104
C	-4.90132493190490	-0.12667659621819	-0.45210063124446
H	-5.54853615725046	-0.24863041154269	0.41780118884136
C	-1.42263302548108	-0.32660809205062	3.40948927779694
H	-0.90965923906967	-0.39835096152398	4.36821283700900
C	-4.66503894573643	0.13876642341729	-2.84742999656283
H	-5.12723074422236	0.22114369817288	-3.83378830079824
C	-3.29438876483827	0.18985758193053	-2.71714841453303
H	-2.63062736569813	0.31058390688473	-3.57489552926670
C	-5.47272791218409	-0.02147137675281	-1.70540289848055
H	-6.55936522371720	-0.06262300593541	-1.80961757928332
C	-2.81815104016606	-0.42358703094114	3.39390639382337
H	-3.35594621564325	-0.56409528987764	4.33407599729057
C	5.03510213190868	0.70998763255351	2.38794405547124
F	5.87053415810790	-0.34108507353459	2.30043147417139
F	5.42684142971913	1.61602395142499	1.49313871039609

F 5.25548726456918 1.24603576512857 3.59315277976539

[2-trifluoromethyl-pBiphe-H]⁺ (**30**), S_{0,eq} in vacuum

N	1.31049835673406	0.00396068648693	-1.36473937589397
C	1.45078801270644	0.05192908707451	1.05828379941658
C	0.75058850923482	0.01150475002793	-0.18383152640253
C	3.49543452441999	0.07853815184991	-0.29391267829005
C	0.74654384612761	0.05679863546085	2.29330465651401
C	2.86653147563886	0.08670044986824	1.00564950568636
C	2.66382880799204	0.03633971035577	-1.45426011435227
C	3.57965000978213	0.12708364411601	2.22211657462957
H	4.66926056487622	0.15456870334203	2.22366636019446
C	4.89238593149697	0.11022033723404	-0.47689504836625
H	5.56393265413992	0.14345424640143	0.38020843797659
C	1.49674481830749	0.09729565412899	3.46314848673848
H	1.00686597250716	0.10286497529998	4.43702088599946
C	4.61223663195762	0.05933186374932	-2.89062015782394
H	5.06503963525747	0.05376526476422	-3.88407521072949
C	3.24753311148400	0.02764648893721	-2.74454548796590
H	2.58091123326030	-0.00430964002814	-3.60743992992768
C	5.43582512946561	0.10046519814789	-1.74406706468488
C	2.89858022289687	0.13200299204540	3.42299693495453
H	3.45681478093379	0.16337812450202	4.36070997268411
N	-1.33200657989649	-0.06166290981484	-1.32155624358548
C	-1.43286771666894	-0.02087625835028	1.05383182541605
C	-0.70643969900598	-0.02470322893691	-0.15783850105775
C	-3.50187935040838	-0.09768003987723	-0.30569152322937
C	-0.72444799477885	0.01955051111566	2.29255974193213
C	-2.85719374179160	-0.05783737120427	0.99329285582670
C	-2.69654626047418	-0.09869166017176	-1.47228528946057
C	-3.56656521245136	-0.05367916852666	2.20462228698735
H	-4.65562953156092	-0.08092026755098	2.21012440783198
C	-4.89886584622869	-0.13604197401984	-0.48674267906036

H	-5.55838306276753	-0.13682221069864	0.38095992386398
C	-1.48286016164699	0.02151629143810	3.45736979721342
H	-0.99871754320867	0.05134281858043	4.43317078333416
C	-4.63050468593363	-0.17306379013691	-2.89351560838242
H	-5.07803072162276	-0.20238675499966	-3.88879656081739
C	-3.25750920447787	-0.13616717199696	-2.75854897149545
H	-2.60475627420047	-0.13571891911773	-3.63436530879413
C	-5.45195424789097	-0.17292351965937	-1.75252417480794
H	-6.53707238941567	-0.20219769193379	-1.86738802385144
C	-2.88196279748301	-0.01466007333817	3.40725913854298
H	-3.44479788146658	-0.01188478824150	4.34319334987750
C	6.93286012121222	0.12902949999764	-1.93860190665613
F	7.58178838075548	0.20048515281978	-0.77802261026216
F	7.34247543551463	-0.96799578119092	-2.57391843486604
F	7.28884697648912	1.17910482437161	-2.67694384884601
H	-0.70147423981132	-0.06065484232133	-2.13236344601082

2-nitro-pBiphe (**31**), S_{0,eq} in vacuum

N	1.31679817547392	0.00405897696957	-1.44510767833416
C	1.44291197865486	0.04736483264738	0.97040643248975
C	0.72750864049747	0.00838850371636	-0.28234798963693
C	3.50448022444707	0.07817680053451	-0.36164920422993
C	0.75189068241138	0.05006614131280	2.21371062521373
C	2.86090851850798	0.08329373274008	0.93291633018922
C	2.67173533265068	0.03747590328624	-1.51490571542290
C	3.57856477060730	0.12207057776447	2.14268840154859
H	4.66837829847325	0.15006651359022	2.13455099361095
C	4.89846457755200	0.11101523154935	-0.53531932165995
H	5.59112889034744	0.14287032729524	0.30444629871225
C	1.50556514436411	0.08928516396977	3.38364100995968
H	1.01302185059008	0.09297882387057	4.35572606078366
C	4.62484497176088	0.06316301898355	-2.96127367724431
H	5.10275682951297	0.05891882198434	-3.94050444515486

C	3.25899796659555	0.03081936910430	-2.80441739109456
H	2.58118617960165	-0.00089149328028	-3.65860871160852
C	5.42662065597919	0.10311375339329	-1.80913489345615
C	2.90313805199630	0.12487713851094	3.34702730746029
H	3.46336546740284	0.15518113546458	4.28407083336797
N	-1.37111601078433	-0.06270605229882	-1.40838484192618
C	-1.43941376760808	-0.02607494697484	1.00647196675819
C	-0.75420109005256	-0.02882335512768	-0.26216346536912
C	-3.53555496994278	-0.10005929183680	-0.27488230193295
C	-0.71986885398585	0.01196497550986	2.23263299309682
C	-2.85830296943832	-0.06264078893945	1.00119928759252
C	-2.72915682597627	-0.09788042901562	-1.44652029199403
C	-3.54358456697145	-0.06098652634376	2.23223152185363
H	-4.63314355200460	-0.08870557384374	2.25242322182763
C	-4.93760111468793	-0.13818628272659	-0.42302331767955
H	-5.58046290724705	-0.14074968445613	0.45839305044177
C	-1.44262589210976	0.01178187324232	3.42178804823449
H	-0.92639928453600	0.03994596677290	4.38117728772920
C	-4.71665502711991	-0.17039211355094	-2.83520853467866
H	-5.18600773868940	-0.19784325598924	-3.82116897339205
C	-3.34446118131241	-0.13358134579100	-2.72025896605998
H	-2.68553648900669	-0.13045071842766	-3.59012163854186
C	-5.51687579292678	-0.17263458522333	-1.67662816291697
H	-6.60502281918355	-0.20182612005247	-1.76837478068786
C	-2.84121155150254	-0.02439708276160	3.41976582410381
H	-3.37886745413229	-0.02350960557640	4.37045306460780
N	6.88552830822320	0.13790372759261	-1.96200068721047
O	7.32632681708131	0.13014590246173	-3.08993567297554
O	7.55634752648717	0.17211203994940	-0.95307989637446

10-nitro-pBiphe (**32**), $S_{0,eq}$ in vacuum

N	1.36176638312598	0.16660936515791	-1.36436888179944
C	1.45853083055587	0.06917907906852	1.04624814675284

C	0.7565502385887	0.08896854784722	-0.21635064510184
C	3.54488374854528	0.07779741782602	-0.26202171475460
C	0.73961235188392	-0.01336179420658	2.27291005880689
C	2.87923709364069	0.16001125705730	1.02048228614339
C	2.71828958881526	0.13477851297700	-1.41972039580181
C	3.52258812498567	0.28505496431909	2.27252034397560
C	4.93141977502109	-0.11936669847671	-0.44667121566304
H	5.59572111786550	-0.27381454317924	0.40121047339308
C	1.45879234958723	-0.00470653650640	3.46515279424103
H	0.95016043231487	-0.08618688724809	4.42449823226125
C	4.66632799083075	-0.02956134861461	-2.85417930165594
H	5.11360277325061	-0.05879049474376	-3.85028495105076
C	3.30466873097036	0.10967541105738	-2.70674405903221
H	2.62667852373459	0.17726063277352	-3.55896093654528
C	5.47797677148069	-0.17060506941495	-1.71377382448453
H	6.55251443963022	-0.33028198660368	-1.82593642119251
C	2.84124351741327	0.15738415533737	3.46579195931408
H	3.39842595928267	0.22184239641360	4.40154516158008
N	-1.32443500267745	0.08530325674798	-1.37915729936486
C	-1.43047303046740	-0.06901038135100	1.02704582389043
C	-0.72485529113776	0.03894058347353	-0.22458404382639
C	-3.50554869112320	-0.08394631858923	-0.28905769414229
C	-0.72943228413130	-0.10638855106277	2.26272396096513
C	-2.84739863542815	-0.13916054864233	0.99622285392546
C	-2.68135876499508	0.03258989113450	-1.44214185403694
C	-3.54813359379260	-0.25829271189391	2.21258889971725
H	-4.63676095659517	-0.31601702650076	2.21341781802523
C	-4.90415102456885	-0.13672189529104	-0.46238835642316
H	-5.55963228959385	-0.22613664119132	0.40518222729931
C	-1.46693874169397	-0.22661784715910	3.43735347716073
H	-0.96656211177514	-0.26334628306416	4.40463045372567
C	-4.64673448303332	0.04140974322408	-2.86398702969711
H	-5.10051935163772	0.08946819606894	-3.85645815525626

C	-3.27720199920779	0.09388151151705	-2.72392555567717
H	-2.60579640334390	0.18295199383913	-3.57956708824017
C	-5.46428675574999	-0.07511355295383	-1.72364242515777
H	-6.55010659233746	-0.11695687588833	-1.83558772613552
C	-2.86324580267331	-0.30379868230786	3.41021706010187
H	-3.41322177533160	-0.39863253209671	4.34897781942766
N	4.92663352046751	0.68128579585719	2.40023340142720
O	5.63204973548075	0.00544590936474	3.11761197854769
O	5.26511479855337	1.68617658592433	1.82014434435767

2-amino-2'-trifluoromethyl-pBiphe (**33**), $S_{0,eq}$ in vacuum

N	1.33683803993489	0.02096540830473	-1.43561598650288
C	1.44390817764916	0.01325951928588	0.97436700462633
C	0.73284633658784	0.00419931080513	-0.27890038459339
C	3.52373085555187	0.06268984778862	-0.34194303360061
C	0.74768098627392	-0.00691707785026	2.21503086328967
C	2.86368361228614	0.04203515068588	0.94577338485198
C	2.68800265604454	0.04922923823445	-1.49423167965526
C	3.56920081987909	0.04827905881476	2.16460885840364
H	4.65928362178681	0.06783422520734	2.16506204210251
C	4.91751974902654	0.09798719964575	-0.50638494555057
H	5.57234341471674	0.10958194297495	0.36697971200377
C	1.49129747283372	0.00113234348352	3.39160543487425
H	0.99062412235599	-0.01410822320160	4.35955908089794
C	4.65761876944563	0.09873985742595	-2.91654731534708
H	5.10868892349566	0.10822878954367	-3.91241387709255
C	3.29410745870971	0.06783162869040	-2.77480566655594
H	2.62817459768868	0.05712473952483	-3.63937156248324
C	5.50149269006627	0.11563908409459	-1.77309720893416
C	2.88944358071702	0.02806465994299	3.36588105343744
H	3.44409021608083	0.03257373784764	4.30680863274116
N	-1.35986252970889	-0.03472527148025	-1.42399302068806
C	-1.43880742181438	-0.04352854467372	0.99305043060770

C	-0.74531068916009	-0.02567065499889	-0.27373946694872
C	-3.52760933347669	-0.07744767171786	-0.29829056413007
C	-0.72463374948502	-0.03541771907110	2.22360779244509
C	-2.85803013398073	-0.07034074486717	0.98272851017028
C	-2.71691841733213	-0.06003469966765	-1.46409694406299
C	-3.55105456861617	-0.08924573255383	2.20806744248737
H	-4.64092609716117	-0.11036578241070	2.22223426864447
C	-4.92833508216757	-0.10105803688279	-0.44738771883015
H	-5.57792077192896	-0.11525635431498	0.42736921921465
C	-1.45545902478028	-0.05489611642368	3.40883748365879
H	-0.94354605156599	-0.04968970127899	4.37086998424468
C	-4.70204929605414	-0.09404776074312	-2.86186610630641
H	-5.17186382651738	-0.10428501942721	-3.84760814569522
C	-3.33308649505152	-0.06972398436521	-2.73956400441273
H	-2.67408147184447	-0.05802569516842	-3.60898868074122
C	-5.50469702469982	-0.10874130127197	-1.70168096698533
C	-2.85334405813771	-0.08161492020523	3.39943741836139
H	-3.39592079018453	-0.09673915702769	4.34732474565781
N	6.86289872411208	0.10864558039024	-1.93316378819207
H	7.23556188450093	0.38455196130308	-2.83048037739876
H	7.43782171821961	0.35463351156284	-1.13990488140301
C	-6.99750942962868	-0.11821350264053	-1.86156383984213
F	-7.43198264188627	1.00196968852791	-2.45214655225146
F	-7.63373616913288	-0.22274419271792	-0.69131719519359
F	-7.40007335364814	-1.13785861912433	-2.62889944932332

2-amino-2'-trifluoromethyl-pBiphe (**33**), $S_{0,eq}$ in chloroform

N	1.33830544373105	0.01938522106546	-1.43474213014577
C	1.44283911980033	0.02479271805760	0.97538989238379
C	0.73146729774111	0.00816869857106	-0.27598084194069
C	3.52543951006451	0.07121146458534	-0.34220480143811
C	0.74694273004604	0.00646198006747	2.21687751063255
C	2.86299179653607	0.06259735747731	0.94614406312384

C	2.68910564770150	0.04654898864137	-1.49671044581019
C	3.56994705923173	0.08942314186497	2.16440763401649
H	4.66010395168345	0.11914964840174	2.16416401421608
C	4.91822889303321	0.10302010030814	-0.50205367439325
H	5.57302430226662	0.12371356366566	0.37100935468298
C	1.49041451353969	0.03878972915714	3.39396449995461
H	0.99159654322416	0.03391248192932	4.36324990524689
C	4.66102977707320	0.08136342133589	-2.91872015665123
H	5.11628149652711	0.08484328193982	-3.91270914902191
C	3.29795862288761	0.05344538027084	-2.77785670927235
H	2.63943656974179	0.03651377539329	-3.64908452704229
C	5.50683525056821	0.10595380750895	-1.77215189705580
C	2.88894128146684	0.08025440954119	3.36614582928384
H	3.44333097733071	0.10470273804651	4.30713684871032
N	-1.36132409538633	-0.01721778774118	-1.42397623134063
C	-1.43882254767253	-0.04981550741772	0.99349156294276
C	-0.74512159156883	-0.01918407098829	-0.27176406065494
C	-3.52840697327734	-0.08254865951856	-0.29959130675784
C	-0.72476446008772	-0.04492645195869	2.22484958431165
C	-2.85843715553965	-0.08825304691226	0.98239169367088
C	-2.71973659569331	-0.04423200952734	-1.46645132520880
C	-3.55290928429571	-0.12921413249859	2.20638323436812
H	-4.64280271646231	-0.16012033300620	2.22027972838841
C	-4.92952777489501	-0.11026988466063	-0.44496559134508
H	-5.57224681903131	-0.14020625305495	0.43466930303014
C	-1.45581200883709	-0.09066031245175	3.41014028777660
H	-0.94612442824796	-0.09639145066933	4.37360981012101
C	-4.70669785921168	-0.06049513569911	-2.86250454407484
H	-5.17538157482773	-0.05241034385458	-3.84934577420594
C	-3.33712974189983	-0.03417601453240	-2.74135738346784
H	-2.68652068814166	-0.00503005031978	-3.61746897567718
C	-5.50606371860128	-0.09895706683291	-1.70023812618661
C	-2.85384960469370	-0.13255691117622	3.39809601751333

H	-3.39620959977742	-0.16779743248779	4.34580043931904
N	6.85694209303721	0.09903269668440	-1.93008666374586
H	7.24617969949086	0.30224386524384	-2.84148201412680
H	7.44993388953385	0.30096711671191	-1.13552662722700
C	-6.99726390496550	-0.11623608662658	-1.85918685366638
F	-7.44280178804170	0.99777976570047	-2.45836212846240
F	-7.63833206608135	-0.21643971835521	-0.69135730162792
F	-7.40088946901988	-1.14263669187959	-2.62112197314571

2-amino-2'-trifluoromethyl-pBiphe (**33**), S_{0,eq} in methanol

N	1.33959367545065	0.02012501303796	-1.43703625975121
C	1.44194287014032	0.02882083302891	0.97344362943775
C	0.73069436073653	0.01016256339210	-0.27727412314876
C	3.52619425236939	0.07564709934414	-0.34274256928883
C	0.74633280899773	0.01031686066578	2.21510300466767
C	2.86210401625254	0.06946456232476	0.94496312096980
C	2.69026070894756	0.04772744960066	-1.49844839516262
C	3.56919450682100	0.10123351488622	2.16293977594294
H	4.65947162887856	0.13387033117530	2.16357135688455
C	4.91824540022245	0.10720989264370	-0.49910003628935
H	5.57220576094699	0.13046640289101	0.37458888281644
C	1.48910584171893	0.04833596328472	3.39257751425900
H	0.99083198956298	0.04518563327656	4.36235056965920
C	4.66497776646100	0.07976374315825	-2.91786644750735
H	5.12226827192524	0.08182643956756	-3.91102897918297
C	3.30224292804080	0.05186701150112	-2.77876008699181
H	2.64862260899433	0.03279932405505	-3.65405216826774
C	5.51030267113930	0.10674470782079	-1.76948589473711
C	2.88751917896048	0.09398089144895	3.36450420658285
H	3.44166930460650	0.12307875538823	4.30567284847243
N	-1.36246834207975	-0.01234654754425	-1.42672353753903
C	-1.43836337447473	-0.05131212689645	0.99120859574160
C	-0.74487468490022	-0.01714471599313	-0.27356330837835

C	-3.52868702789430	-0.08424407716428	-0.30075431391293
C	-0.72451114382877	-0.04715937709176	2.22277358395471
C	-2.85804158589343	-0.09308873109057	0.98076276353268
C	-2.72172570188610	-0.04027287558538	-1.46816461567151
C	-3.55265612668408	-0.13982492021845	2.20418394925477
H	-4.64261429922975	-0.17346454917021	2.21913667854417
C	-4.93006922820543	-0.11352756808644	-0.44310621187915
H	-5.56944910006576	-0.14781167697003	0.43894648066403
C	-1.45504392713207	-0.09961362653935	3.40823188670910
H	-0.94602523069839	-0.10774061842961	4.37222409405277
C	-4.71127702720142	-0.05287081647332	-2.86105034006382
H	-5.17969658582493	-0.04048937164089	-3.84819447037646
C	-3.34146192711651	-0.02549381230902	-2.74172977023622
H	-2.69603583323657	0.00829372663860	-3.62180461904203
C	-5.50834793002896	-0.09759058586161	-1.69761142164060
C	-2.85287669642793	-0.14571099506147	3.39568072686609
H	-3.39502202198253	-0.18609312769721	4.34347143653720
N	6.85564268526731	0.10465160291890	-1.92496556605573
H	7.25353718531004	0.26497297011193	-2.84150799971967
H	7.45592370766009	0.27326661465979	-1.12761075335495
C	-6.99906058501827	-0.11641629351485	-1.85465116114706
F	-7.44737429462709	0.99886127273344	-2.45092123833816
F	-7.64010354499433	-0.22055582962646	-0.68751449366044
F	-7.40299790997934	-1.14140093658967	-2.61946632420587

2-amino-2'-trifluoromethyl-pBiphe (**33**), $S_{0,eq}$ in dimethyl sulfoxide

N	1.33900014233721	0.02231564095081	-1.43590611782161
C	1.44206824904136	0.02905453565360	0.97463277455786
C	0.73066346045443	0.01108277352444	-0.27612028057012
C	3.52589688183046	0.07692136592109	-0.34233782255347
C	0.74636430826890	0.00996565089781	2.21620547006782
C	2.86217231169788	0.06962704193992	0.94568764062916
C	2.68920031461120	0.05022011261121	-1.49808357586991

C	3.56945900808372	0.10035522794549	2.16353787301186
H	4.65968165061523	0.13286815606207	2.16354757979059
C	4.91763797155514	0.10831181619824	-0.49938796941424
H	5.57225083782913	0.13047955237195	0.37378970026795
C	1.48939737359250	0.04689466532521	3.39355204099367
H	0.99103245422769	0.04305999244677	4.36320540607466
C	4.66279524647539	0.08348498340198	-2.91902270374614
H	5.12017954787935	0.08657161897022	-3.91201532974353
C	3.30026843699103	0.05560412403066	-2.77908486239479
H	2.64503264718788	0.03733182021677	-3.65311557318725
C	5.50900773549584	0.10914886324528	-1.77064995818708
C	2.88785617138450	0.09222410275040	3.36519915412176
H	3.44207788189190	0.12042979250259	4.30619163824715
N	-1.36213051728632	-0.01310765716514	-1.42559510273243
C	-1.43866634769882	-0.05104732774869	0.99246559784650
C	-0.74510021012109	-0.01706350420634	-0.27243940577409
C	-3.52855578390922	-0.08432861360090	-0.30018506058741
C	-0.72462264987584	-0.04685978465056	2.22389723626512
C	-2.85829747905109	-0.09265183274283	0.98162220631375
C	-2.72105152217736	-0.04121178870760	-1.46765890206729
C	-3.55305245160314	-0.13881994276385	2.20494008241276
H	-4.64296175849689	-0.17225185922504	2.21932471617124
C	-4.92977397712523	-0.11339978240965	-0.44332830474802
H	-5.56974821289414	-0.14692015771137	0.43831583408799
C	-1.45536656962899	-0.09870439241925	3.40925935407912
H	-0.94622880873680	-0.10658373031062	4.37311993974014
C	-4.70966645030460	-0.05453549078923	-2.86162684654593
H	-5.17834157550754	-0.04281389982603	-3.84856428271784
C	-3.33991212143540	-0.02730472192989	-2.74183040725851
H	-2.69298999930985	0.00578669283295	-3.62075413994599
C	-5.50703133799392	-0.09819483076728	-1.69833943309244
C	-2.85324466680831	-0.14439846622558	3.39648093600018
H	-3.39537773758982	-0.18426425089612	4.34414275074836

N	6.85314892116252	0.10904155203901	-1.92690772913529
H	7.25332618838701	0.25614962096582	-2.84450648839447
H	7.45685444681308	0.26386390386579	-1.12951736264262
C	-6.99748944683384	-0.11698133902802	-1.85639516779812
F	-7.44503510709229	0.99668143337547	-2.45613644688162
F	-7.63940569791189	-0.21776005182272	-0.68957032389510
F	-7.40122175842088	-1.14377161509880	-2.61883833372233

2-amino-2'-trifluoromethyl-pBiphe (**33**), $S_{0,eq}$ in water

N	1.34227130513073	0.01615920751942	-1.44222102849378
C	1.44120858373084	0.02843919082083	0.96842697109931
C	0.73095192305423	0.00850091662496	-0.28277876288596
C	3.52711379415062	0.07327257839615	-0.34395344460504
C	0.74603226883323	0.01098840601795	2.21008435865053
C	2.86118091321796	0.06922920942536	0.94214559762265
C	2.69394984147986	0.04319069465780	-1.50083120288278
C	3.56781790228925	0.10294995095689	2.16024683452768
H	4.65781244541566	0.13576090728276	2.16010319598804
C	4.91963129493387	0.10501211545151	-0.49600463934439
H	5.57081105242474	0.13062402322569	0.37946253690560
C	1.48754504782185	0.05104446384611	3.38815394996390
H	0.98751042137517	0.04894741550349	4.35671954120365
C	4.67334685376937	0.07311991910863	-2.91387844031950
H	5.13424747491789	0.07401581692310	-3.90501195345561
C	3.31014246945505	0.04532071658113	-2.77891523374337
H	2.66165234229365	0.02525706977856	-3.65735189569061
C	5.51498948351447	0.10187028061166	-1.76385740651793
C	2.88583486994371	0.09734152211054	3.36150024907603
H	3.43910205353772	0.12807353354248	4.30261694200721
N	-1.36443489284618	-0.01082510153460	-1.43199841102018
C	-1.43721817376768	-0.05192336955211	0.98596583327501
C	-0.74457341977186	-0.01729602795542	-0.27909866471546
C	-3.52901965500706	-0.08423272419453	-0.30248151250555

C	-0.72400348150514	-0.04781098186608	2.21764935551308
C	-2.85670188325602	-0.09406579727482	0.97753113215011
C	-2.72462309787593	-0.03846378725821	-1.47086217384746
C	-3.55101234138395	-0.14180409787154	2.20097935068973
H	-4.64069689247809	-0.17563213832244	2.21509522236440
C	-4.93075969816370	-0.11399646526400	-0.44048464562796
H	-5.56738039058962	-0.14997036836173	0.44330185039356
C	-1.45344800734704	-0.10141503065871	3.40357960284879
H	-0.94287465609609	-0.10978916781875	4.36644484452924
C	-4.71827594430667	-0.04948761104931	-2.85824807269599
H	-5.18993442905902	-0.03579914661135	-3.84347259630398
C	-3.34820079358234	-0.02189000367951	-2.74235482279842
H	-2.70761438805844	0.01333191231260	-3.62526223394342
C	-5.51217819319178	-0.09635231923056	-1.69311316744150
C	-2.85113033091871	-0.14826976379832	3.39227116715429
H	-3.39246417181231	-0.18951388861965	4.33997411544870
N	6.86211816450326	0.09606285537051	-1.91568890631371
H	7.25379494849911	0.28075931219831	-2.83031424723625
H	7.45158818997000	0.29021426005787	-1.11613960656962
C	-7.00279668084412	-0.11559035477015	-1.84646032687354
F	-7.45278527575431	1.00043012219409	-2.43963458093177
F	-7.64063348902930	-0.22230299203702	-0.67812514227458
F	-7.40779335761678	-1.13898526278956	-2.61250953237313

2-amino-2'-nitro-pBiphe (**34**), $S_{0,eq}$ in vacuum

C	-7.27509073098088	-2.69077705377488	-0.02264918001908
C	-5.90606288701402	-2.56216824228561	-0.02719021616224
C	-5.29061664473545	-1.28527034407135	-0.01469446603265
C	-6.10140463692517	-0.11542725400523	0.00279209542331
C	-7.49845466628309	-0.26003821299720	0.00726514581456
C	-8.05441905760497	-1.52259718663436	-0.00526225120573
C	-5.43114160213831	1.16617561023929	0.01508073749669
C	-4.01215137406299	1.17447981151680	0.00889682307565

C	-3.31995699767026	-0.09333455220262	-0.00930011303589
C	-3.29667683495077	2.40398719722683	0.02038384832750
C	-4.02766168906382	3.58957860586085	0.03770082934229
C	-5.42545536684122	3.58110099866826	0.04375610590240
C	-6.12467011831834	2.38999280576736	0.03269914319702
H	-7.77261204321832	-3.66014782590791	-0.03203511118307
H	-5.24576419698672	-3.43046464849003	-0.04053744009378
H	-8.17355334271889	0.59443956289846	0.02038673130480
H	-3.51547845575333	4.55142366276320	0.04685879082557
H	-5.96759023339644	4.52918651422349	0.05738138852400
H	-7.21478741079244	2.40358083814675	0.03765591242948
C	-1.84279186732019	-0.09925722713172	-0.01598719653244
C	-1.13010513622964	1.15256025443360	-0.00357115358477
C	0.10995198930116	-1.31850044989622	-0.03957615987534
C	0.28984345516934	1.12161872926483	-0.00976774247358
C	-1.82458211604345	2.39404472190633	0.01386798814264
C	0.71382387226749	-2.60063995236876	-0.05774330698053
C	0.94803177538873	-0.16705477848811	-0.02736479839129
C	0.99712995709273	2.33940170729807	0.00045045259201
C	-1.07932784537876	3.56951119684187	0.02407396215298
C	2.07696192107267	-2.74474904445769	-0.06330227809320
H	0.04620861999930	-3.46390240395162	-0.06639874274746
C	2.34141847683662	-0.33412243992709	-0.02991370020118
C	0.31905274294465	3.54173351484015	0.01714304807509
H	2.08733520851534	2.33839981463397	-0.00594009806739
H	-1.57850655379883	4.53828290605177	0.03722892989852
C	2.92315382731893	-1.60240738251109	-0.04832984969365
H	2.52658266773419	-3.74108272232314	-0.08177392788484
H	2.99822685919041	0.53770936212130	-0.02011805996350
H	0.87504744293041	4.48177925668921	0.02458783601805
N	-3.93514324717463	-1.24466153384678	-0.02016674027197
N	-1.24033389141786	-1.25756415159315	-0.03332982722600
N	4.28217379785432	-1.76400168064175	-0.09088996435765

H	4.86754324958775	-0.97534702883771	0.14448640941361
H	4.66320219579486	-2.66822342620707	0.14804899638442
N	-9.51487400447611	-1.64477785890694	-0.00015049341297
O	-10.16635375343525	-0.62221293030209	0.01489334076111
O	-9.98012135426863	-2.76345673963227	-0.01134569761149

10-amino-10'-trifluoromethyl-pBiphe (**35**), S_{0,eq} in vacuum

N	1.34560539987128	-0.01410119629533	-1.36835638645241
C	1.44193216580586	0.08300516042793	1.04136176883173
C	0.74169237973382	0.00149634650684	-0.21664485851103
C	3.52625464271324	-0.00075090982133	-0.25375364429296
C	0.70565761157344	0.09823451585558	2.25264147431323
C	2.86068891558460	0.18644390454335	1.01938630715838
C	2.70153825920851	-0.05246324052404	-1.41704726039651
C	3.53042322476422	0.49308382406560	2.24563748582089
C	4.91653435418773	-0.20383729166866	-0.43485493952030
H	5.56932709646158	-0.30537459685664	0.43020797530403
C	1.41681125804928	0.28834488488322	3.43571245574245
H	0.89901993637409	0.32042717501566	4.39441844342012
C	4.64978936612114	-0.32738728593388	-2.84174517956459
H	5.09274060642053	-0.43940711617303	-3.83387078158743
C	3.28705966125248	-0.18558739377479	-2.69716943610344
H	2.60451870585708	-0.19622702719011	-3.54862780950132
C	5.46198420684085	-0.36392121158323	-1.69606071166587
H	6.53659638023323	-0.53478511181538	-1.79533134715460
C	2.78699300231714	0.50485764043097	3.42823540003922
H	3.30140530213400	0.71876564672845	4.36882617790106
N	-1.32059520842403	-0.01868126955844	-1.39248328019987
C	-1.47186336377662	-0.07466358785743	1.01662747567383
C	-0.74337340866592	-0.01698465545507	-0.22817851119951
C	-3.52448490109603	0.02602544738300	-0.32007722133773
C	-0.74961717324557	-0.07473975254139	2.24323352545170
C	-2.89717954444401	-0.17218004130936	0.97789839430674

C	-2.67373375704582	0.04112433387518	-1.46485372655633
C	-3.56274443486686	-0.46677292261519	2.20623845540804
C	-4.89944068962115	0.26946643952523	-0.53904984539588
H	-5.58148944129255	0.37995304632260	0.29639659744681
C	-1.46582317442767	-0.25440897743621	3.42087742195060
H	-0.95980791217123	-0.27891343136030	4.38516826314383
C	-4.57678763782652	0.34717806294816	-2.94025822695343
H	-4.99431099364720	0.45767449438881	-3.94366302148679
C	-3.22415564072721	0.16824481099783	-2.76207641184278
H	-2.51996480868769	0.14700548484075	-3.59529173186169
C	-5.41183808872856	0.42411100184701	-1.81257146198951
H	-6.47957152339217	0.61875805112315	-1.93626925379563
C	-2.83578564460610	-0.48408045969758	3.38836847246437
H	-3.35065323491643	-0.71326063509037	4.32093242433747
N	4.87613482972291	0.77606406266048	2.30227115022146
H	5.27554295179250	1.22656705834861	1.48794986905811
H	5.18708113015943	1.18817458136809	3.17286572247889
C	-5.01054723356535	-0.87962591036250	2.34185859902965
F	-5.22833541972691	-1.50134402528131	3.50640391651403
F	-5.86138389182554	0.16403980525945	2.32545360464806
F	-5.39214426045183	-1.72554772914435	1.38466366670489

10-amino-10'-nitro-pBiphe (**36**), S_{0,eq} in vacuum

N	-0.94237955077224	1.59402211921743	-0.01966879128620
C	-0.84725867356560	1.62090329461594	2.39415702655490
C	-1.54595952917684	1.57219024249535	1.13209846669919
C	1.23712027762777	1.57014728249666	1.09377588557707
C	-1.58015506787388	1.60910232465609	3.60992833283853
C	0.57225471324267	1.71972905902649	2.37227621692759
C	0.41303358017876	1.55982960505776	-0.07087237418559
C	1.24733627329425	1.98690268973374	3.60548424422584
C	2.62661148990600	1.36726862311288	0.90567004220694
H	3.27924159342650	1.23160933946754	1.76613136220233

C	-0.86165184885278	1.75196610279055	4.79578510383299
H	-1.37354234410088	1.74935907007049	5.75800831162205
C	2.36007167582702	1.33032283384452	-1.50450017721336
H	2.80314768792617	1.25207395522636	-2.49975148845373
C	0.99783747064453	1.47040955387484	-1.35520632328529
H	0.31520630236041	1.49030660091333	-2.20641125810943
C	3.17150769992765	1.24979562109100	-0.36039925526359
H	4.24536888934767	1.07791551667929	-0.46548031962253
C	0.50912201295152	1.95916135981709	4.79136052606779
H	1.02844799252420	2.13470648795543	5.73709209069728
N	-3.61747734651134	1.54517705151143	-0.04105176453982
C	-3.74676627270055	1.44827275846292	2.36722662608490
C	-3.02904538379703	1.53312491376706	1.11910221785412
C	-5.81446962301872	1.51545162031786	1.03872879770149
C	-3.03710886310485	1.45929467872317	3.60238736317282
C	-5.16428398406973	1.32996877729158	2.31839466033778
C	-4.97332315637486	1.57366610543613	-0.10879007825168
C	-5.81699744318645	1.08768142520260	3.54897512628042
C	-7.20116011694921	1.71326046351554	0.85441521327478
H	-7.87672908387167	1.77747148386950	1.70494039862610
C	-3.76774480093136	1.33118596882841	4.78344369368650
H	-3.26943384474152	1.34057559048232	5.75176172923751
C	-6.90653383300240	1.85104378798420	-1.54710174984293
H	-7.34212829660150	1.96790083662343	-2.54202388047287
C	-5.5459099593332	1.71153919089746	-1.39552789082373
H	-4.85690258709800	1.72830787789997	-2.24169537960903
C	-7.73348223684470	1.87695293148147	-0.40893496268793
H	-8.80848695099811	2.03472045552902	-0.51961454644904
C	-5.14381189726650	1.13240192286110	4.75463838087737
H	-5.70678936987111	0.97348730573680	5.67551237260962
N	-7.20793477310579	0.64368857563858	3.63303608310967
O	-7.92084791785683	1.19597427212161	4.44417126197705
O	-7.53451304179946	-0.28121424873020	2.92503087513069

N	2.59170719084144	2.26792011193736	3.66653566170889
H	2.99425089060063	2.73370121759635	2.86264878350715
H	2.90894309335019	2.65082324287145	4.54801338546721

2-amino-10¹-trifluoromethyl-pBiphe (**37**), S_{0,eq} in vacuum

N	1.31345227689395	-0.16268736440387	-1.42557754033697
C	1.41611294507455	0.08166208233034	0.96731134142239
C	0.70672745169661	-0.06994880371525	-0.27415155145225
C	3.49728533302278	0.05097861454663	-0.34289165813011
C	0.71250782091142	0.15687434307288	2.19829851487431
C	2.83343089974372	0.15850028584858	0.93789175720222
C	2.66470854542062	-0.11626824580241	-1.48539803692085
C	3.52784804806372	0.33463856399074	2.15015167842702
H	4.61628610923997	0.39931368974990	2.15212922936570
C	4.89041974082621	0.10340048926262	-0.50959826355612
H	5.54156395577471	0.23175487352409	0.35725618110562
C	1.44365920672842	0.34062417603076	3.36888970929860
H	0.93764028061081	0.42226309774685	4.33058498595457
C	4.63756891041680	-0.18349028243083	-2.90263982234897
H	5.09131447924080	-0.27894861104368	-3.89277508356468
C	3.27451833658059	-0.23117444406078	-2.75901696543644
H	2.61207175963946	-0.35757888951065	-3.61705308056389
C	5.47765229420713	-0.01196028947436	-1.76941773765376
C	2.83918134767049	0.43102886153219	3.34312585183647
H	3.38499382554270	0.57619538445532	4.27794677128316
N	-1.36943645038176	-0.19501949938783	-1.41939690931732
C	-1.48628579853499	-0.04602717942246	0.98965459524158
C	-0.77304515965135	-0.09823980215901	-0.26851726788466
C	-3.55730987645337	-0.02356803499506	-0.32844381244003
C	-0.75456577334612	0.03407663843711	2.20820630663475
C	-2.91438713829924	-0.12056848989511	0.97352036204126
C	-2.72265716263229	-0.12654075364261	-1.47978922519032
C	-3.57102564498899	-0.30116631534586	2.22836204632291

C	-4.93035573216235	0.22735888118573	-0.55012840403686
H	-5.59735509830951	0.42839654468946	0.28065397472124
C	-1.46158920672397	-0.02385637370201	3.40218876313604
H	-0.94740918018589	0.02997693786894	4.36059392214792
C	-4.64242345361410	0.07740090990100	-2.95156177489275
H	-5.07249916851313	0.10307172082472	-3.95546409079659
C	-3.29034686108872	-0.10934908141728	-2.77558018273199
H	-2.59895754729655	-0.21833079375401	-3.61266145711807
C	-5.45938549903806	0.27481115403859	-1.82543712139774
H	-6.52489481804360	0.47907117322871	-1.95246877012848
C	-2.83612750978257	-0.22749873441859	3.40250813058909
H	-3.34621135094461	-0.36444145732767	4.35549852247454
N	6.83997145239167	-0.00405852445983	-1.92743827680142
H	7.20675709808364	0.17920461516269	-2.85061099232150
H	7.40395166259393	0.35280917695044	-1.16911853282222
C	-5.02396501437971	-0.68149057841897	2.41185307537468
F	-5.23480231475331	-1.20609607992676	3.62443064555494
F	-5.85910738898569	0.37031423286427	2.32329193721425
F	-5.42748063226478	-1.59501781852772	1.52978825562074

2-amino-10¹-nitro-pBiphe (**38**), S_{0,eq} in vacuum

N	1.31792180966563	-0.11150089849272	-1.43021216132841
C	1.41983942933184	0.05672231458343	0.97152377556755
C	0.71140773315422	-0.05611587113225	-0.27609588220717
C	3.50160333156286	0.05576031529752	-0.34165838983453
C	0.72039525283678	0.10490777785532	2.20837015406722
C	2.83828525564210	0.11984209788487	0.94263346600003
C	2.66841415900278	-0.06427108083834	-1.48978267903725
C	3.53764044996152	0.24029470841188	2.15890589812717
H	4.62677512325519	0.29049239399152	2.15995756762535
C	4.89467159798028	0.10728424120413	-0.50687926579773
H	5.54716913033411	0.19970335835738	0.36343425071194
C	1.45800719669420	0.22657267529025	3.38308269798840

H	0.95662899572818	0.27030073528860	4.34962381992222
C	4.63984537546431	-0.08580158999423	-2.90986705354146
H	5.09298365089028	-0.14508428729878	-3.90305496309277
C	3.27694366919233	-0.13305369736318	-2.76752641113649
H	2.61360527917755	-0.22427409437308	-3.62930198637441
C	5.48099861665153	0.03774920063107	-1.77085659813167
C	2.85441075545479	0.29535145381922	3.35741204751085
H	3.40481731859546	0.39062602659634	4.29586551662154
N	-1.37472880386628	-0.18630123834562	-1.41771432366133
C	-1.46863438989712	-0.06800952966699	0.99311767092342
C	-0.76631360370412	-0.10109254314606	-0.27060269549123
C	-3.55644738718413	-0.07603988158299	-0.31315743265255
C	-0.74883539706121	0.02059721510369	2.21898268287005
C	-2.88998336551917	-0.15256554214536	0.96932250546465
C	-2.73093333777933	-0.14708021313339	-1.47065420059638
C	-3.53319053322819	-0.26559784978631	2.22249380546477
C	-4.94206405403690	0.12890692997064	-0.49706787482305
H	-5.60318277867547	0.29457320963934	0.35130178477955
C	-1.46808688805755	0.02593744008757	3.41212863369136
H	-0.95858368632333	0.11352444666004	4.37045494301228
C	-4.68174640190790	0.01752746041188	-2.90310274577481
H	-5.13000356264949	0.04117138062076	-3.89902400473144
C	-3.32074179066009	-0.12926489705041	-2.75656376553341
H	-2.64483656186553	-0.20836014228671	-3.60948687904960
C	-5.49134516723320	0.17355343647066	-1.76312966550345
H	-6.56497955620348	0.33951208525721	-1.87483382546759
C	-2.85051974992136	-0.13016830017923	3.41473317995654
H	-3.40790576837277	-0.18455711521677	4.35098878171062
N	-4.93761817002637	-0.65729162207189	2.35532452885207
O	-5.63875620756893	0.02080663438755	3.07545228199747
O	-5.28266216614734	-1.66166109972666	1.77784088265635
N	6.84218390688073	0.04613334912375	-1.92900810388939
H	7.21225130370085	0.25487117739456	-2.84530754707641

H 7.41099998673173 0.36336942949176 -1.15696242078884

10-amino-2'-trifluoromethyl-pBiphe (**39**), S_{0,eq} in vacuum

N 1.36152002413234 0.18937129988701 -1.35943355437902
C 1.46606025949890 0.03749271623988 1.05185475309962
C 0.76293113697445 0.08678089321974 -0.20942567829328
C 3.54496690813778 0.06315412756356 -0.26116053813157
C 0.73925356139290 -0.05166795311670 2.26864814027152
C 2.88802600429666 0.11980072882605 1.02942769205840
C 2.71665345147667 0.15175229228910 -1.41925253577145
C 3.57405448125263 0.27841891098606 2.27446584964674
C 4.93163586989047 -0.13737808890799 -0.47189260061601
H 5.58584176020760 -0.34485210436178 0.37278304742374
C 1.46650181928741 -0.01193743669816 3.45568759064306
H 0.95792805870956 -0.07861592158332 4.41753315848536
C 4.65535347114904 0.01879188920492 -2.87634358502391
H 5.09360016000450 0.01562302225985 -3.87682524976102
C 3.29510207772103 0.15875622743063 -2.70951054976410
H 2.60889879185447 0.25148267322107 -3.55301796333380
C 5.47028433671391 -0.15943297959482 -1.74592492460659
H 6.54217446219905 -0.33187203742636 -1.86918122715594
C 2.84181415318860 0.17073592444463 3.45806924602239
H 3.36888888429158 0.26395762619324 4.41135539786213
N -1.31625026807406 0.12830893440624 -1.37777256023423
C -1.42828878643719 -0.09722160309836 1.02528831382132
C -0.72074314709323 0.04673278065128 -0.22095657887720
C -3.49624634975707 -0.07937668009947 -0.29454287129183
C -0.72368255488325 -0.16512047173204 2.25886765224169
C -2.84540760553109 -0.17415962348573 0.99202144659670
C -2.67196855921719 0.07632720993214 -1.44075338570330
C -3.54985618503920 -0.33752402608659 2.19968707456213
H -4.63801582193908 -0.40241462271131 2.19855872186467
C -4.89378428852639 -0.13016750983957 -0.46796293588720

H	-5.55329337281997	-0.24939092336789	0.39115616387713
C	-1.46550734674830	-0.33520372242195	3.42625243555384
H	-0.96444906685909	-0.40860608262270	4.39142944875699
C	-4.63645090580074	0.12762725301168	-2.86609677732957
H	-5.09348010991410	0.20599571800997	-3.85477367705122
C	-3.27064485118799	0.17804353662472	-2.72049352295462
H	-2.60112078746875	0.29577393962856	-3.57384174359897
C	-5.45272848447637	-0.02846999338727	-1.72576128035525
C	-2.86075149436349	-0.42104332568841	3.39382115307384
H	-3.40989755734567	-0.55498363241505	4.32862075564138
N	4.92690352132223	0.52972066602251	2.34917555150526
H	5.32320599933792	1.07114412081183	1.59040825990682
H	5.24756701924593	0.83902086849932	3.25813180032359
C	-6.94203724655452	-0.07809448996566	-1.91167704188711
F	-7.40104527408736	1.04829760119220	-2.47006126248259
F	-7.59355627978023	-0.24524709923888	-0.75747734922614
F	-7.29885986838132	-1.08193063270619	-2.72150425952241

10-amino-2'-nitro-pBiphe (**40**), S_{0,eq} in vacuum

N	1.35963301962579	0.16222677476190	-1.36164676907790
C	1.46340116175067	0.04947033280024	1.05204529155319
C	0.76102686224691	0.07940968313576	-0.20976749551204
C	3.54211737901848	0.04980606667503	-0.26091729946678
C	0.73637388180486	-0.01920218180127	2.26980120377248
C	2.88547116551368	0.12879644446724	1.02823419567938
C	2.71419526280399	0.12140142191697	-1.42090223646847
C	3.57177334174872	0.30593361735215	2.27106298591831
C	4.92833150625739	-0.15711036243432	-0.46851135327458
H	5.58239123101179	-0.35265745136826	0.37908687686938
C	1.46364128925811	0.03667632054309	3.45633113405558
H	0.95497016045790	-0.01484058256591	4.41905044019700
C	4.65224643276356	-0.03851840440966	-2.87565320522751
H	5.09084795929528	-0.05855576187651	-3.87572455471339

C	3.29246578778740	0.10678059548909	-2.71138729754950
H	2.60652926113377	0.18739630834258	-3.55633626069952
C	5.46649944248905	-0.20063297309509	-1.74209866606004
H	6.53793854417873	-0.37761113386689	-1.86262955385604
C	2.83914307393657	0.21668762965153	3.45624243956465
H	3.36621440114397	0.32307521483325	4.40808338447520
N	-1.31589103253132	0.10530459439287	-1.38221344847644
C	-1.43018714840413	-0.08068880283065	1.02606453743109
C	-0.72217329304915	0.04147722748982	-0.22225629493355
C	-3.49621743228663	-0.08169938978710	-0.29577853969996
C	-0.72625357791172	-0.12919590045454	2.26083675405863
C	-2.84711171137150	-0.15593710040110	0.99393991898452
C	-2.67009863158962	0.05446915894072	-1.44708211401454
C	-3.55399935436526	-0.29732020903139	2.20154163829013
H	-4.64232419221247	-0.36012639469968	2.19925974332392
C	-4.88995491679785	-0.13356006702406	-0.46610815608706
H	-5.57612367673020	-0.23708531718509	0.37321251650885
C	-1.47043917359298	-0.27761316276726	3.43021572649448
H	-0.97071513740546	-0.33502893799179	4.39713216040449
C	-4.63109870319513	0.08694483489174	-2.88393909166824
H	-5.11420955739625	0.14824579407348	-3.85867443853268
C	-3.26554732984505	0.13699131937211	-2.73062310755648
H	-2.59333698708512	0.24030297842635	-3.58360963476257
C	-5.42590107628392	-0.04961842287246	-1.73411382568159
C	-2.86538596141200	-0.36132505177541	3.39787609665352
H	-3.41574896055905	-0.47784942714976	4.33422531034732
N	-6.88375977840970	-0.10487432224809	-1.88328743085879
O	-7.33138743750727	-0.02725897805457	-3.00626675038927
O	-7.54908506208707	-0.22434503027121	-0.87697177775598
N	4.92378898388910	0.55744330808689	2.34194200766317
H	5.32362865734623	1.08296953014317	1.57407391951346
H	5.24742132656694	0.87694621017605	3.24624102056411

5-*N*-oxide-pBiphe (**41**), S_{0,eq} in vacuum

N	1.42043615712484	-0.04434200034465	-1.41650417049751
C	1.45376320455654	0.08724131824499	0.99125115841637
C	0.76956805868513	0.02476056691758	-0.28690065097839
C	3.57158050180575	0.09090243275659	-0.27115943927350
C	0.73791200157175	0.08455194359414	2.21556949558651
C	2.87394876134531	0.15091170900265	0.99406797689913
C	2.77753917199246	-0.03047996893855	-1.44030452426920
C	3.55048356043325	0.25773118481784	2.22266986316517
H	4.63885384216315	0.31361644898511	2.24216356087445
C	4.97416388684334	0.12951013173183	-0.40716157518418
H	5.60770935646651	0.22721359671134	0.47575314188037
C	1.45241129295582	0.20362746652913	3.40791704849988
H	0.93030781934639	0.23269758625311	4.36358667913051
C	4.77865801606239	-0.09157006728609	-2.81043767449732
H	5.25715988549932	-0.16284168671098	-3.78997080674026
C	3.40484979463537	-0.12406160401077	-2.70528820740924
H	2.75296446943320	-0.21567238944450	-3.57565341876483
C	5.56752205536322	0.03937656990623	-1.65217103035906
H	6.65635980198929	0.06923774583362	-1.73585676616370
C	2.84451760951095	0.29427968284659	3.40942664195306
H	3.37694502797426	0.38840399890812	4.35850558461227
N	-1.37678055560003	0.12634203535383	-1.46304115382162
C	-1.42520265994220	-0.06108441699476	0.95527820792749
C	-0.69915701651510	0.03220272974647	-0.28458990574073
C	-3.54141166474681	-0.12862665845409	-0.29603940675620
C	-0.72175976253220	-0.05355545754989	2.19530178727170
C	-2.84275860497421	-0.15706328751758	0.97049534425469
C	-2.80121734688972	0.02579076652154	-1.47786425335368
C	-3.52601721096369	-0.27050731866410	2.18952867352940
H	-4.61305185390633	-0.34594003993849	2.19882875503427
C	-4.94275562687658	-0.23489899175188	-0.42093157563117
H	-5.55513170402194	-0.35943538600497	0.47195639639850

C	-1.44619222307369	-0.17907162595095	3.38115067928258
H	-0.92168504002513	-0.19804548610917	4.33561310920059
C	-4.79531691741458	-0.02363317347329	-2.82164335060893
H	-5.28277216013065	0.01657064571202	-3.79800190068628
C	-3.42141989676117	0.08220534924211	-2.73402601884070
H	-2.78239224908932	0.20652087628050	-3.60658389060801
C	-5.55971194524452	-0.18446901074919	-1.65606417864676
H	-6.64658649564193	-0.27010868826789	-1.72156969127783
C	-2.83393952156889	-0.28937060509950	3.38580475591706
H	-3.37056861342878	-0.38707017564382	4.33149861197276
O	-0.83054045641074	0.29441604800976	-2.56287551669765

2-dimethylamino-5'-*N*-oxide-pBiphe (**42**), $S_{0,eq}$ in vacuum

N	1.34362038396767	-0.12430367304778	-1.51420368588713
C	1.43679597308842	0.21602064513614	0.86821131415226
C	0.71657713184541	0.02946596417590	-0.37694114185271
C	3.52523746810835	0.14364545550846	-0.44794823937954
C	0.75580222083288	0.31071876231125	2.10930649419816
C	2.85626377626255	0.30017036940971	0.82708935852766
C	2.69354911249763	-0.08712246980098	-1.57319793052174
C	3.56213363751505	0.52173865751111	2.02315737151932
H	4.64973935885592	0.59431877754913	2.00770829851429
C	4.91767859770580	0.19661122186700	-0.61290964040222
H	5.54552990622524	0.37835937397545	0.25605805717946
C	1.49957084395056	0.54257710842703	3.26676969124927
H	1.00228261838388	0.64724219728370	4.23039319592412
C	4.66869785261324	-0.22501326655671	-2.98670656211186
H	5.09658370318320	-0.37186671516310	-3.97775451151261
C	3.30532370880871	-0.27121958523659	-2.83581125658533
H	2.64377401771405	-0.44748051886163	-3.68583831086033
C	5.51826484866291	0.01674920662359	-1.86725078353510
C	2.88949840661367	0.65149155378895	3.22265036583165
H	3.44576610055600	0.83452215871540	4.14474490722102

N	-1.46272365224539	-0.02190409507677	-1.49445880895687
C	-1.43951583499115	0.01975834376867	0.93025569983619
C	-0.74968433639096	0.00758825567615	-0.33391076508416
C	-3.58913000632505	-0.19593633855740	-0.24563084050496
C	-0.70187812086355	0.15243775722255	2.14359582132990
C	-2.85470643985385	-0.09446290452897	0.99663385185136
C	-2.88352539744575	-0.14424176722322	-1.45743862436304
C	-3.50169729692443	-0.10199147049023	2.24045944964203
H	-4.58674629356971	-0.19104664945908	2.28830960613491
C	-4.99131364119551	-0.33370566428611	-0.31886280410498
H	-5.57634053592670	-0.38143210615572	0.59950662349465
C	-1.39129166766511	0.12885521919789	3.35668297549917
H	-0.84028651539894	0.20674521092280	4.29304066150091
C	-4.91409943104300	-0.35026001752975	-2.73156793849556
H	-5.42876739545762	-0.41035740117382	-3.69293879656227
C	-3.54021796190585	-0.21699458852997	-2.69435528041367
H	-2.92622471220514	-0.16715158479809	-3.59200414140090
C	-5.64365630092259	-0.41014263783570	-1.53447585383572
H	-6.73035531832250	-0.51736732325448	-1.55962753082071
C	-2.77636289557946	0.00118159561052	3.41244387450225
H	-3.28468997441922	-0.01412237388960	4.37858187460659
O	-0.94931343459557	0.04729733922787	-2.62335449374074
N	6.88147456984079	0.06939091203618	-2.02294749139260
C	7.47413119175317	-0.12941440671501	-3.31946104832649
H	7.14028426773070	0.62647988025518	-4.05271791850172
H	8.56455050769509	-0.04856453038488	-3.23411986802251
H	7.24482338176218	-1.12619312345734	-3.73764877723847
C	7.72027500757574	0.30843557223630	-0.88028264687063
H	7.60915681536493	-0.47691715431533	-0.10993495267620
H	8.77084552673564	0.32251405913223	-1.19452382449447
H	7.49969622739754	1.27909676875914	-0.39967502425984

2-dimethylamino-5'-*N*-oxide-*p*Biphe (**42**), $S_{0,eq}$ in chloroform

N	1.33782213237584	0.06783327056011	-1.52345732373224
C	1.44070082427218	0.10456874379875	0.88219614658159
C	0.71418994033849	0.04093780773406	-0.37126244608974
C	3.52837865798717	0.12759922344161	-0.44102638252747
C	0.76288942503703	0.16143292498752	2.12826267929704
C	2.86340270916344	0.11607943537075	0.84697832378245
C	2.68766015046426	0.12592217618041	-1.58523987530306
C	3.57916144053515	0.13020784591462	2.05822843435065
H	4.66952019265703	0.13203793792302	2.04756699179510
C	4.92120167100246	0.15571987479943	-0.59921293808909
H	5.55388649495702	0.15352354876432	0.28538515971409
C	1.51540085018265	0.16393442403045	3.30374867632232
H	1.02324983710051	0.18241789179091	4.27572885045438
C	4.65956362911596	0.20391249195320	-3.01250202371261
H	5.08248119558775	0.23749460761068	-4.01621878954474
C	3.29565879547081	0.16821674168171	-2.86401357788474
H	2.63727525175711	0.16953090547254	-3.73564439441126
C	5.51944176740307	0.19300873670843	-1.87135668710119
C	2.91043837845761	0.14150378948970	3.26756855985953
H	3.47354880723659	0.14198104133662	4.20377432225427
N	-1.46364275551224	-0.26596725963708	-1.45704267119172
C	-1.44247960956603	0.12326907428677	0.93353015590181
C	-0.75139006203038	-0.03725987107090	-0.32166113963575
C	-3.59723908059473	0.01917086036204	-0.24958762983772
C	-0.70218266399834	0.23301343981664	2.14715849897642
C	-2.86215778559779	0.16400001201663	0.98811880021120
C	-2.88594799600628	-0.21093532659068	-1.43828574198304
C	-3.51444092373138	0.33253941152191	2.21899868666186
H	-4.60327148039456	0.36158216107552	2.26017118388810
C	-5.00448193852123	0.08114258295602	-0.33511919358703
H	-5.59188755065628	0.26529408715849	0.56455736776692
C	-1.39516247337254	0.40798082433724	3.34660953616741
H	-0.84596937442477	0.51072286780261	4.28190727978896

C	-4.92440118305739	-0.32367136504015	-2.71463161053449
H	-5.43974835982238	-0.45592797671569	-3.66871380596081
C	-3.54536408900764	-0.38728477101181	-2.66422563200874
H	-2.93847823917266	-0.56614533171454	-3.55008369619985
C	-5.65779973652823	-0.08571476779137	-1.54180495092765
H	-6.74826991589132	-0.03154693094831	-1.57870111124348
C	-2.78638378487833	0.46009455032831	3.38751656557007
H	-3.29815278231976	0.59757208884846	4.34245163138955
O	-0.94017103838406	-0.52334382389532	-2.56159454944409
N	6.87659412482867	0.22051784495283	-2.02113897513386
C	7.46701709971539	0.28632978999549	-3.33582844077245
H	7.17575363754315	1.20202457560237	-3.88054963621920
H	8.55921470374660	0.28827312851436	-3.23947688776516
H	7.18838032690802	-0.58054069315076	-3.95977135864442
C	7.72553476347644	0.23182430276090	-0.85693116341837
H	7.57124089998300	-0.66124332027942	-0.22582606701760
H	8.77540113890726	0.24132912355706	-1.17239615212113
H	7.55313787425761	1.12166990640355	-0.22467782869101

2-dimethylamino-5'-*N*-oxide-pBiphe (**42**), $S_{0,eq}$ in methanol

N	1.34061757108956	0.07454693960870	-1.52390566700397
C	1.44054313986179	0.10045825297769	0.88047699144493
C	0.71424104256731	0.03995200023571	-0.37172941912102
C	3.53008800281820	0.12842691033908	-0.44101160715621
C	0.76349399393982	0.15717298015140	2.12663133248780
C	2.86331805141599	0.11109995265543	0.84593976569438
C	2.68952371329007	0.13406387757338	-1.58652203253228
C	3.57937314431655	0.12032865192100	2.05700796804439
H	4.66993587169159	0.12083551097092	2.04747832631307
C	4.92182373680638	0.15531733158433	-0.59721059227305
H	5.55424128835349	0.14648789243118	0.28768418740010
C	1.51507335703538	0.15564480476199	3.30230286888777
H	1.02343045412847	0.17472713875207	4.27472682763829

C	4.66168991240320	0.21773751804809	-3.01304852219733
H	5.08518028485833	0.25631483490462	-4.01649062323282
C	3.29847701756220	0.18301205260263	-2.86542066187928
H	2.64381981325553	0.19023055820873	-3.74019962868668
C	5.52136829561429	0.19946598308796	-1.87030843806048
C	2.91029235792813	0.12938546244129	3.26620903244521
H	3.47325787941896	0.12634380823250	4.20258585100334
N	-1.46762482504710	-0.27460480397419	-1.45297320494377
C	-1.44159337240302	0.12556219169506	0.93161930679643
C	-0.75221181391068	-0.04075902022080	-0.32502157516464
C	-3.59660531408402	0.02132700477691	-0.25124517277755
C	-0.70076605902883	0.23510377475847	2.14454826198952
C	-2.86071864837072	0.17044640623794	0.98470658851868
C	-2.88585815472454	-0.21987293875195	-1.43892891402332
C	-3.51332131196011	0.34535347322119	2.21501400878156
H	-4.60205674348478	0.37785537166440	2.25791311073566
C	-5.00367145780935	0.08788383035001	-0.33313583292915
H	-5.58868508871672	0.28162763064368	0.56609439793322
C	-1.39279760488408	0.41565760102719	3.34335479084655
H	-0.84481326206088	0.51776707610047	4.27957659304972
C	-4.92921225443444	-0.33694333503228	-2.70856764524359
H	-5.44699376003541	-0.47598886488841	-3.66055417956279
C	-3.55029452252186	-0.40436587331331	-2.66210689413918
H	-2.95606307910217	-0.59187432102725	-3.55426918629303
C	-5.66000603767916	-0.08658074036126	-1.53679476254940
H	-6.75042992079526	-0.02904803050494	-1.57247712148553
C	-2.78405289206287	0.47363267413976	3.38231901612548
H	-3.29549138323729	0.61571920173413	4.33694652722326
O	-0.94038234414462	-0.54186521835622	-2.56638957678430
N	6.87498429739926	0.22636315424340	-2.01886559987856
C	7.46821207389443	0.29167752439375	-3.33419371419567
H	7.17655253774759	1.20728546530479	-3.87791974936445
H	8.56001714205279	0.29488731422458	-3.23534248392957

H	7.19086542678100	-0.57615269250022	-3.95690619093941
C	7.72522723557568	0.22663372615205	-0.85337040007539
H	7.57141367851918	-0.67292443538777	-0.23201640300615
H	8.77462893364345	0.24077386832625	-1.16953706887076
H	7.55108349352917	1.11050313783585	-0.21419771506005

2-dimethylamino-5'-*N*-oxide-pBiphe (**42**), S_{0,eq} in dimethyl sulfoxide

N	1.33740770203314	0.07301157927693	-1.52614285444437
C	1.44026728027076	0.10360292632752	0.88000516287408
C	0.71327665748589	0.04227695518495	-0.37348768290155
C	3.52883764525192	0.12798124364472	-0.44262582412270
C	0.76300678342069	0.16059388316680	2.12645691848199
C	2.86300397413468	0.11406561245552	0.84529475819283
C	2.68748061808264	0.13091061710725	-1.58725483497395
C	3.57953740476865	0.12606797700039	2.05599663144763
H	4.67004599160124	0.12697209004683	2.04590812218456
C	4.92130726200698	0.15494944782393	-0.59862963633555
H	5.55334968293574	0.14873313784278	0.28663660251561
C	1.51547095220898	0.16185070114903	3.30207042625841
H	1.02394957364776	0.18175593807514	4.27447499141525
C	4.66172619362769	0.21213222676228	-3.01335614972368
H	5.08542793917161	0.24905425860574	-4.01676636197640
C	3.29781703160610	0.17732687864138	-2.86537001372672
H	2.64324344014088	0.18298015264116	-3.74018310545830
C	5.52156726745106	0.19640070982325	-1.87116623655175
C	2.91050141588755	0.13728154013891	3.26545512039425
H	3.47371646553409	0.13665119009893	4.20160355325773
N	-1.46460945696118	-0.26958171132504	-1.45753789111496
C	-1.44222142366031	0.12492987429808	0.93246344843774
C	-0.75195079869369	-0.03731584524087	-0.32315935099250
C	-3.59726608276519	0.02025197356640	-0.24971377702733
C	-0.70175794275285	0.23450126605935	2.14582021425359
C	-2.86169982424638	0.16708181780648	0.98740517955287

C	-2.88663403679193	-0.21470867236154	-1.43808246785220
C	-3.51401735365648	0.33768012181923	2.21805047808927
H	-4.60290476278078	0.36795402841120	2.26045700032363
C	-5.00450234225525	0.08385131655392	-0.33346405964200
H	-5.59111018403402	0.27226389876056	0.56589800164992
C	-1.39382283207436	0.41087853840179	3.34566668985505
H	-0.84502579213731	0.51242298947802	4.28148299924511
C	-4.92685261789862	-0.33092784439829	-2.71163150387959
H	-5.44392458146561	-0.46723836834527	-3.66430452008962
C	-3.54771405285723	-0.39563528403813	-2.66268796880780
H	-2.94389401359603	-0.57909471504768	-3.54958861811428
C	-5.65883306731631	-0.08702064108190	-1.53910901141256
H	-6.74928213915960	-0.03175351960670	-1.57552075962496
C	-2.78507999631466	0.46516914109222	3.38619782069395
H	-3.29647677436293	0.60394174633075	4.34117525059255
O	-0.94051796508547	-0.53056650466090	-2.56206406907962
N	6.87584006272857	0.22357233383856	-2.01941630142338
C	7.46854697362235	0.28786566629102	-3.33403544938524
H	7.17665611251330	1.20302429100157	-3.87868295625341
H	8.56029554161104	0.29003290020331	-3.23491791191756
H	7.18926523256131	-0.57952267081966	-3.95664375920234
C	7.72477293530899	0.22727499523417	-0.85403721415331
H	7.56848352081982	-0.66945289252795	-0.22907454021262
H	8.77423871647613	0.23905158566405	-1.16994811156890
H	7.55018156095656	1.11310373282980	-0.21744125774687

2-dimethylamino-5'-N-oxide-pBiphe (**42**), $S_{0,eq}$ in water

N	1.33331101456997	0.06860631838284	-1.52896035962407
C	1.43954309204550	0.05906093816602	0.87617816109025
C	0.71188659337347	0.01096996010236	-0.37429132609396
C	3.52520026021017	0.07481680376678	-0.44759876014223
C	0.76408600854099	0.12721692603837	2.12256331318312
C	2.86153484348758	0.05228408964933	0.84035607642989

C	2.68377332844003	0.11909217019972	-1.59181006345325
C	3.57868208296681	0.04571333502613	2.05092197266482
H	4.66891619774119	0.03236627042697	2.03957381778302
C	4.91702444424450	0.07185000378851	-0.60416118617100
H	5.54891857041550	0.02529616544907	0.27987797911122
C	1.51552250001290	0.11136390428103	3.29777398746033
H	1.02312669814419	0.13911242896527	4.26947862550604
C	4.65768130492580	0.19308208769294	-3.01679547840028
H	5.08223511230488	0.23918432671919	-4.01922823535824
C	3.29408599463324	0.18409400367733	-2.86919314226188
H	2.64218071793754	0.21840523874078	-3.74475819728792
C	5.51686160643577	0.13555277592741	-1.87560028765452
C	2.91037871759538	0.06065679094833	3.26055131676660
H	3.47362575699329	0.04600318981272	4.19613859746491
N	-1.46925154311264	-0.35313409899835	-1.44040225590062
C	-1.44034437491373	0.12075695105536	0.92921858274096
C	-0.75317494065508	-0.07689034975142	-0.32311343990376
C	-3.59408341265287	0.01742279575047	-0.25270369725645
C	-0.69787934114249	0.23615600587734	2.14004467981603
C	-2.85816783899055	0.18557285523756	0.98047609573148
C	-2.88640236833234	-0.27557625184872	-1.43064374625387
C	-3.50812754835654	0.39381642447257	2.20700091433013
H	-4.59613726508740	0.44273999394199	2.24820179572472
C	-4.99916437260920	0.10977592573069	-0.33932908176457
H	-5.58001332697513	0.34498889089599	0.55246861308423
C	-1.38629478444464	0.44807161177300	3.33544321729405
H	-0.83537829749908	0.55411440168834	4.26935714651724
C	-4.92985330005482	-0.39506032434614	-2.69923390590240
H	-5.44880272715681	-0.55469205178286	-3.64684401193582
C	-3.55255796994688	-0.48849713760093	-2.64786514792150
H	-2.96087149965295	-0.71659223153341	-3.53185185332707
C	-5.65712270383126	-0.09085825405879	-1.53802458388698
H	-6.74562014487743	-0.01203732188422	-1.57814083543110

C	-2.77663812070255	0.53158162523697	3.37203997738289
H	-3.28571739894270	0.69892119614070	4.32334384716373
O	-0.94267193430517	-0.67998417861615	-2.54031950877468
N	6.87177786734626	0.14298083887674	-2.02433207310133
C	7.46399034734742	0.10969891744504	-3.34244963386225
H	7.15544166212778	0.97458471198610	-3.95153332314129
H	8.55491096612740	0.14629465486849	-3.24480787786946
H	7.20259030246448	-0.80852543132211	-3.89734336166930
C	7.72000662916078	-0.00463942722203	-0.86543539710943
H	7.55661436510976	-0.96749655604516	-0.34909413006789
H	8.76932930808585	0.04023412362734	-1.17757492415137
H	7.55278818245380	0.80220089364449	-0.13291682256717

2,2'-N-oxide-pBiphe (**43**), $S_{0,eq}$ in vacuum

N	1.34707618705760	0.03369486535943	-1.41819188643970
C	1.44038174439181	0.03777083484792	0.99821549721912
C	0.73733715109630	0.01883502113254	-0.26160236958147
C	3.51865925245641	0.09141457453006	-0.30288695531913
C	0.73582244912508	0.01969764028634	2.23401007924869
C	2.85971358259823	0.07514315507490	0.98407385461927
C	2.69501514208243	0.06869770573744	-1.45955996968935
C	3.56157140513934	0.09455551693350	2.20303197390561
H	4.65150644673283	0.12326525889178	2.20950414329027
C	4.90620595038037	0.12771248343868	-0.45675978720768
H	5.62348354626520	0.14742394194797	0.36135968766953
C	1.47395599307722	0.04026158114816	3.41457451922137
H	0.96833472789258	0.02774469029221	4.37989788629633
C	4.70184316614276	0.11980969928369	-2.80886132038330
H	5.27537827493421	0.13383367319880	-3.73464750443899
C	3.34215590206596	0.08427546660299	-2.71972408131217
H	2.72670548329286	0.06719195994778	-3.62002399556908
C	2.87165686686523	0.07732676758466	3.39913829840137
H	3.41901880651860	0.09261430226607	4.34395229080791

N	-1.34716909910946	-0.03380235420369	-1.41809059088630
C	-1.44029338650702	-0.03784668646752	0.99832405616016
C	-0.73734326851639	-0.01892740501026	-0.26154695410399
C	-3.51866841726813	-0.09150685308538	-0.30262202732098
C	-0.73564153044011	-0.01975773832459	2.23406546921756
C	-2.85962637286586	-0.07521907515602	0.98428920324489
C	-2.69511109485024	-0.06880534326888	-1.45935715837938
C	-3.56139270790045	-0.09461575930958	2.20330021518249
H	-4.65132721377922	-0.12332531160674	2.20985446309826
C	-4.90622669779448	-0.12780607486940	-0.45639004018431
H	-5.62344270657817	-0.14750639833895	0.36178374052810
C	-1.47368641974644	-0.04030662864542	3.41468568546383
H	-0.96799295380485	-0.02777746067340	4.37997097676261
C	-4.70204073543265	-0.11993402474720	-2.80850692047287
H	-5.27564587616797	-0.13396969305886	-3.73424958263344
C	-3.34234673733802	-0.08439919473985	-2.71947231236433
H	-2.72696408191223	-0.06732755088170	-3.61981869116392
C	-2.87138843306592	-0.07737189609074	3.39935461902149
H	-3.41868035456821	-0.09264742795868	4.34420932227117
O	6.74418836731852	0.17472280778806	-1.79634264706711
O	-6.74430985239051	-0.17483278092824	-1.79583393969518
N	-5.50130609271012	-0.14219778121617	-1.67564624488925
N	5.50119358731291	0.14208849228828	-1.67606100252810

2,2'-*N*-oxide-pBiphe (**43**), $S_{0,eq}$ in chloroform

N	1.34670522121266	0.02773684202960	-1.41794554754216
C	1.44044002059455	0.04245471621068	0.99888541252824
C	0.73792932054904	0.01766202868371	-0.25966416384715
C	3.51720646518521	0.09174073600900	-0.30415055184479
C	0.73567305773993	0.02740568412804	2.23485117909714
C	2.85994630385776	0.08533342033250	0.98381383464978
C	2.69697407726853	0.06070646748969	-1.46229113707824
C	3.56343799647362	0.11953649797027	2.20180893499134

H	4.65341714526566	0.15353570827881	2.20799721503582
C	4.90557621440987	0.12500659988460	-0.45629280518306
H	5.61448936827101	0.14961938511782	0.36961978364779
C	1.47358578237105	0.06681579550265	3.41557689965736
H	0.96964889711807	0.06434201850698	4.38205691156848
C	4.70461616448440	0.09807866419402	-2.80724327921811
H	5.27215141897870	0.10315649369860	-3.73735763982545
C	3.34390675517066	0.06546632356270	-2.72159586073011
H	2.73868316012212	0.04201716917807	-3.62919240874885
C	2.87175813636033	0.11241860302327	3.39763500781608
H	3.41872589928232	0.14221779374483	4.34260069048986
N	-1.34679881698802	-0.02784538143358	-1.41784311458891
C	-1.44035194958743	-0.04253117438346	0.99899470875321
C	-0.73793570721318	-0.01775552250227	-0.25960795694263
C	-3.51721639124447	-0.09183259006004	-0.30388480906302
C	-0.73549205915001	-0.02746669593386	2.23490723289932
C	-2.85985944732625	-0.08540911966199	0.98403015945749
C	-2.69707082748295	-0.06081468522106	-1.46208720095083
C	-3.56325964285741	-0.11959610838535	2.20207856252210
H	-4.65323830411259	-0.15359399516355	2.20834949415219
C	-4.90559751849006	-0.12509904256995	-0.45592312859802
H	-5.61444995451870	-0.14970022950915	0.37004182140936
C	-1.47331602117376	-0.06686170089102	3.41568905030720
H	-0.96930688262772	-0.06437629256511	4.38213150714994
C	-4.70481294596823	-0.09820312036520	-2.80688915624450
H	-5.27241749021860	-0.10329292481491	-3.73696115410071
C	-3.34409719990972	-0.06559094593481	-2.72134365729042
H	-2.73894068303330	-0.04215465639388	-3.62898525625826
C	-2.87148980266289	-0.11246378553669	3.39785258016877
H	-3.41838669410846	-0.14225080760130	4.34285971420611
O	6.74795277076953	0.15774136576887	-1.79227046327264
O	-6.74807376653033	-0.15784864973318	-1.79176287031929
N	-5.49668422705309	-0.12832935915331	-1.67333741837803

N 5.49657215677215 0.12822147449896 -1.67375112048242

2,2'-N-oxide-pBiphe (**43**), S_{0,eq} in methanol

N 1.34564137098788 0.01943594735123 -1.41951883433197
C 1.43986685719670 0.04675328887418 0.99811607208243
C 0.73873503936383 0.01608213132031 -0.25998969659863
C 3.51419098991074 0.09282270508412 -0.30443892004803
C 0.73505369966903 0.03348550799243 2.23364783914308
C 2.85900808058032 0.09504359571793 0.98333727251415
C 2.69759017013705 0.05157222964672 -1.46364399364923
C 3.56302497840417 0.14177022879457 2.20030032034308
H 4.65290471314572 0.18162139674350 2.20751656630572
C 4.90316395192985 0.12529203678540 -0.45547966541490
H 5.60933710431893 0.15637532273452 0.37319611093931
C 1.47206620103810 0.08634434910096 3.41410788007934
H 0.96863173863903 0.08864753726523 4.38101574194113
C 4.70613251628546 0.07769524114158 -2.80420762622467
H 5.27242317094785 0.07464005338556 -3.73543242874283
C 3.34467902128716 0.04554278970648 -2.72166725220275
H 2.74518898646312 0.01411219893547 -3.63286344519984
C 2.87014877320147 0.14055004448458 3.39540437963849
H 3.41651702362592 0.18139248062749 4.34043023407479
N -1.34573526471895 -0.01954581016386 -1.41941636877253
C -1.43977884984551 -0.04682978874236 0.99822543208723
C -0.73874152886794 -0.01617600833616 -0.25993335606582
C -3.51420104619628 -0.09291424612100 -0.30417332081389
C -0.73487274553860 -0.03354640916423 2.23370390468512
C -2.85892129573482 -0.09511926733902 0.98355371214167
C -2.69768715740697 -0.05168145180686 -1.46344009337353
C -3.56284669856119 -0.14183037774582 2.20057025551044
H -4.65272578980490 -0.18168103529377 2.20786943003418
C -4.90318529169998 -0.12538262787162 -0.45511023859196
H -5.60929767442922 -0.15645244532569 0.37361766683885

C	-1.47179646849293	-0.08639032153253	3.41422007826498
H	-0.96828958351550	-0.08868189344038	4.38109033578874
C	-4.70632913866390	-0.07782002326031	-2.80385377517666
H	-5.27268901945607	-0.07477695608178	-3.73503654029415
C	-3.34486947547321	-0.04566896702161	-2.72141530107263
H	-2.74544651698526	-0.01425252053301	-3.63265611091054
C	-2.86988048289037	-0.14059581940528	3.39562220217884
H	-3.41617783375461	-0.18142663720020	4.34068955615082
O	6.75235202598986	0.14641031323362	-1.78656295474269
O	-6.75247279682404	-0.14651363070916	-1.78605523198030
N	-5.48906909569656	-0.11786018500444	-1.66976347159846
N	5.48895734143458	0.11775402317321	-1.67017636493641

2,2'-N-oxide-pBiphe (**43**), S_{0,eq} in dimethyl sulfoxide

N	1.34708843046212	0.02240936059959	-1.41887646078202
C	1.44019551943182	0.04520369462139	0.99811823837336
C	0.73798993999521	0.01657655891492	-0.25992633023923
C	3.51710842853591	0.09215060925903	-0.30442211297213
C	0.73529986717687	0.03156557712383	2.23390458084873
C	2.85959277039263	0.09154828779076	0.98319625415017
C	2.69790896823881	0.05467618313524	-1.46305889022499
C	3.56297574921169	0.13426726136839	2.20078778844011
H	4.65292484987845	0.17198256296056	2.20735298871705
C	4.90560329188767	0.12475145905057	-0.45471665611732
H	5.61090850438655	0.15332465405234	0.37436320557021
C	1.47237766492813	0.08048435446358	3.41477106641724
H	0.96846345896484	0.08179585913527	4.38138752544147
C	4.70680067576805	0.08471106883224	-2.80564240009204
H	5.27306930473510	0.08483255890590	-3.73659744210811
C	3.34607774533197	0.05254143619483	-2.72152142850902
H	2.74472972149244	0.02411294825668	-3.63173652792345
C	2.87046378029687	0.13167139525096	3.39628846668998
H	3.41696875661628	0.16920451658048	4.34126405464752

N	-1.34718242749507	-0.02251510094843	-1.41877361146838
C	-1.44010766792997	-0.04527848633273	0.99822773607395
C	-0.73799651758609	-0.01666732646568	-0.25986988204133
C	-3.51711868073169	-0.09224198182903	-0.30415604886585
C	-0.73511901668256	-0.03162504229788	2.23396073687394
C	-2.85950612825501	-0.09162323915370	0.98341287712239
C	-2.69800602269307	-0.05478274234661	-1.46285457559523
C	-3.56279745201750	-0.13432719848506	2.20105786354967
H	-4.65274597095698	-0.17204229619601	2.20770607397741
C	-4.90562476924558	-0.12484520419622	-0.45434700625192
H	-5.61086964268059	-0.15340788190442	0.37478452051801
C	-1.47210785935368	-0.08052961543544	3.41488340718642
H	-0.96812114690884	-0.08182973816614	4.38146218586376
C	-4.70699711993225	-0.08483623182264	-2.80528827220896
H	-5.27333454853805	-0.08497037285239	-3.73620139099739
C	-3.34626806754591	-0.05266472651940	-2.72126896821866
H	-2.74498700717313	-0.02424806162192	-3.63152866520834
C	-2.87019537848079	-0.13171689832229	3.39650641116761
H	-3.41662945362875	-0.16923872848938	4.34152351457187
O	6.75001751968768	0.14983659900834	-1.79011779803871
O	-6.75013822245743	-0.14994883427600	-1.78961076574842
N	-5.49780134004426	-0.12128229871686	-1.67131539370683
N	5.49768949291810	0.12117206087334	-1.67172886888254

2,2'-*N*-oxide-pBiphe (**43**), $S_{0,eq}$ in water

N	1.34797589628213	0.01622439975782	-1.42382107524183
C	1.43878901746491	0.04779706379909	0.99397028035187
C	0.73872253472604	0.01548390660599	-0.26455403316186
C	3.51450537216179	0.09327086669504	-0.30483178349806
C	0.73458704149307	0.03477049830071	2.22957565459586
C	2.85766434369947	0.09730985188701	0.98135132608581
C	2.70080406459316	0.04849575902226	-1.46511152625603
C	3.56138757775237	0.14641853628863	2.19824067597917

H	4.65096605192725	0.18722510038528	2.20438433327015
C	4.90371827120594	0.12677215792592	-0.45091378045869
H	5.60582827225670	0.16073013591503	0.38067489728440
C	1.47044460407000	0.09002408317029	3.41051340361456
H	0.96529024304313	0.09264240723525	4.37622107419949
C	4.71361506459294	0.07255950473659	-2.79937368607057
H	5.28137971245331	0.06738817780859	-3.72918085079319
C	3.35213020670513	0.03950322175875	-2.72070125332702
H	2.75789935301787	0.00519925766042	-3.63463414526676
C	2.86834274181477	0.14608199769155	3.39310087407386
H	3.41380097862775	0.18881588151893	4.33805524569470
N	-1.34807002884825	-0.01633764254722	-1.42371846926231
C	-1.43870137051219	-0.04787569841852	0.99407960554422
C	-0.73872932448494	-0.01558115546901	-0.26449770046768
C	-3.51451548629811	-0.09336275048837	-0.30456606081116
C	-0.73440640245432	-0.03483317483686	2.22963170064216
C	-2.85757781246026	-0.09738646533571	0.98156779722859
C	-2.70090111311249	-0.04860690239517	-1.46490737210308
C	-3.56120954249726	-0.14647863162683	2.19851072786722
H	-4.65078747303678	-0.18728395179322	2.20473773089349
C	-4.90373933624950	-0.12686062025644	-0.45054431955614
H	-5.60578857925533	-0.16080326144784	0.38109610420777
C	-1.47017514127078	-0.09007067573153	3.41062556467489
H	-0.96494844142021	-0.09267684581254	4.37629548960292
C	-4.71381123750975	-0.07268345145109	-2.79901939654989
H	-5.28164496379200	-0.06752360942609	-3.72878446472565
C	-3.35232044800862	-0.03963085268596	-2.72044882415753
H	-2.75815671518698	-0.00534233486160	-3.63442594441919
C	-2.86807463038892	-0.14612762816055	3.39331873901963
H	-3.41346197304087	-0.18884899518646	4.33831463747263
O	6.75901310014511	0.14617372431010	-1.77641954914711
O	-6.75913318883306	-0.14627157731240	-1.77591139208502
N	-5.49358483160650	-0.11666419295451	-1.66304353614509

N 5.49347359223426 0.11656088572465 -1.66345669879953

2-dimethylamino-2'-*N*-oxide-pBiphe (**44**), S_{0,eq} in vacuum

N 1.24510231754943 -0.12619385213719 -1.54857093071306
C 1.42360271705403 0.15605041949391 0.84176095142108
C 0.67539152206612 -0.01505511836409 -0.37865572917478
C 3.46277533614622 0.08056635039087 -0.53753249939467
C 0.76506885210266 0.27379647742020 2.09745206441884
C 2.84115585578163 0.20538417972217 0.76455057772342
C 2.59286359071333 -0.08291471618788 -1.65112498761084
C 3.58101219172494 0.37301867486712 1.95075119624628
H 4.66996322760632 0.41366259857735 1.91460692736567
C 4.85027211205103 0.11291455107300 -0.74283406392732
H 5.50617616503060 0.23737481685703 0.11539459329916
C 1.54243655409484 0.43837583675495 3.24070738078088
H 1.07147385955337 0.53245050062653 4.21907020184992
C 4.52434004030520 -0.17428286416431 -3.12824778691602
H 4.92062182384199 -0.27371096450293 -4.13806705550287
C 3.16630730383262 -0.20764095295893 -2.93915074776995
H 2.47943500441015 -0.33186239320015 -3.77822473612159
C 5.41105059074235 -0.01136623575645 -2.02230729921496
C 2.93783438778939 0.48743462894207 3.16712331420839
H 3.51998330457616 0.61756854131430 4.08210184673200
N -1.45124656541605 -0.22453438034910 -1.44328464731047
C -1.45497418608228 0.05113408125976 0.95926092011132
C -0.79765472148160 -0.06890058026110 -0.32135154338985
C -3.57974437109587 -0.17512008979476 -0.24497664911712
C -0.70506391317735 0.21951037706731 2.15689738781576
C -2.87337246305039 -0.00208667602139 1.00503056193400
C -2.79996527211077 -0.27843487491051 -1.42640196820396
C -3.52961040878401 0.11330875943400 2.24366849685634
H -4.61815377941771 0.07497044259241 2.29454413960204
C -4.97199751637862 -0.24414407044649 -0.33947989479090

H	-5.65682001837794	-0.17610192693787	0.50350920773059
C	-1.39966306491634	0.32832940516067	3.35956606340212
H	-0.85803296692374	0.45731529652827	4.29638286494878
C	-4.85705193152879	-0.50814467139310	-2.67988569005888
H	-5.46407227841556	-0.63626657222997	-3.57504271520730
C	-3.49495516680270	-0.44775632306849	-2.64890896916541
H	-2.91391376698058	-0.52913215655012	-3.56839218743286
C	-2.79582630307617	0.27604777571999	3.40235710201349
H	-3.30761890627264	0.36507487256196	4.36308083921847
N	-5.61310004515485	-0.40693319178396	-1.52326241206899
N	6.76828806623280	0.02138995118086	-2.21554676748634
C	7.31978976233038	-0.11412541655963	-3.53898889719600
H	6.98695491389717	0.69295744446531	-4.21579346540693
H	8.41378707985977	-0.06729355734455	-3.48026801863732
H	7.05180484305868	-1.07798294458233	-4.00725975373742
C	7.64515224482783	0.18848851816724	-1.08782663644473
H	8.68605410797992	0.19671529205266	-1.43245076207520
H	7.45887242752940	1.13892033487472	-0.55546725073716
H	7.53937452125822	-0.63150235775473	-0.35418953135773
O	-6.86130707850275	-0.46687323984465	-1.59012304150785

2,2',10,10'-tetra-*N*-oxide-pBiphe (**45**), $S_{0,eq}$ in vacuum

N	1.35065061381346	0.03573754675625	-1.39076483533807
C	1.44040646405432	0.03827339406323	1.01990297390918
C	0.73625213980972	0.01950168507590	-0.23770323450088
C	3.53856952152146	0.09397257937370	-0.27684803858922
C	0.72598402045598	0.01931587275393	2.24336444884439
C	2.85567397439849	0.07591331069128	0.99207553080225
C	2.69445579271092	0.07143210753771	-1.43192921635667
C	4.92702548600829	0.13087645825525	-0.45617214404105
H	5.63665466147260	0.14982082443055	0.36292406169610
C	1.48830967612265	0.03968589784574	3.41293073063663
H	1.02487323524088	0.02743978773152	4.39918833903536

C	4.67558746252423	0.12395914062154	-2.81560843278574
H	5.23249893677173	0.13867169836107	-3.75159861922985
C	3.31935838876226	0.08791996165228	-2.70145754972719
H	2.68427758584858	0.07095578377711	-3.58765947837366
C	2.86262794620465	0.07627621897755	3.36399482844373
H	3.51047244498487	0.09359671809569	4.23924892699706
N	-1.35076301276960	-0.03584135132366	-1.39065282121495
C	-1.44032008725376	-0.03833568796100	1.02002246615053
C	-0.73626948760955	-0.01958561292476	-0.23764212107218
C	-3.53859014628534	-0.09405707768235	-0.27655448021190
C	-0.72579679835697	-0.01935700128448	2.24342476589851
C	-2.85558979606470	-0.07597608452464	0.99231249371734
C	-2.69457160481120	-0.07153645144821	-1.43170568724708
C	-4.92706084437621	-0.13096393014550	-0.45576346457389
H	-5.63662243099484	-0.14989454007195	0.36339159799605
C	-1.48802581692215	-0.03970671611561	3.41305433707340
H	-1.02450798556270	-0.02744300863557	4.39927349594410
C	-4.67581746830987	-0.12408685338949	-2.81522051885566
H	-5.23280583291153	-0.13881540517477	-3.75116468539293
C	-3.31957894431975	-0.08804603589596	-2.70118209331744
H	-2.68457152678004	-0.07109732272646	-3.58743690208047
C	-2.86234814281109	-0.07629793645543	3.36423238397072
H	-3.51012086908285	-0.09360317292828	4.23953990258680
N	3.55852880650106	0.09470627053095	2.19252056490288
N	-3.55834558102221	-0.09474899025987	2.19281589650136
N	-5.48973184009891	-0.14582361176566	-1.69520521839172
N	5.48959420233090	0.14571523746923	-1.69566051776855
O	4.80862549080618	0.12798341536538	2.23000516927842
O	-4.80843912022353	-0.12802657336357	2.23040417600253
O	-6.72754326886476	-0.17873166611462	-1.83901952274889
O	6.72739375508833	0.17862112082595	-1.83957750856939

2,2',10,10'-tetra-*N*-oxide-pBiphe (**45**), $S_{0,eq}$ in chloroform

N	1.34876820449547	0.02755035168370	-1.38913814641488
C	1.44003942958794	0.04472388831577	1.02177536111001
C	0.73678939458447	0.01829850494917	-0.23495640933893
C	3.53464874306908	0.09574669318755	-0.27705652506069
C	0.72638590380951	0.02804267393591	2.24465058766275
C	2.85483053480236	0.08915023546694	0.99362300738717
C	2.69515816876897	0.06148088674071	-1.43316670950722
C	4.92317760195323	0.12953407855995	-0.46008955387110
H	5.63045889897948	0.15647707402678	0.36067044632219
C	1.48655356559123	0.06897793841050	3.41475743993207
H	1.02610963025312	0.06744342777858	4.40251585273098
C	4.67658911902178	0.09624621874436	-2.81562672134415
H	5.22623276319014	0.09915737201760	-3.75649911629467
C	3.31928285004831	0.06358409398065	-2.70202383882136
H	2.69267742371679	0.03763543517701	-3.59452696493230
C	2.86068541399193	0.11600743391501	3.36263139065983
H	3.50056395743704	0.14941763780878	4.24386764539549
N	-1.34888095838987	-0.02765431971756	-1.38902561725738
C	-1.43995297284559	-0.04478519605614	1.02189527279153
C	-0.73680664965483	-0.01838180568453	-0.23489487614538
C	-3.53466963832462	-0.09583115026499	-0.27676284635566
C	-0.72619853625692	-0.02808231405698	2.24471126666074
C	-2.85474631775979	-0.08921306780833	0.99386044391974
C	-2.69527443659534	-0.06158573389931	-1.43294275016094
C	-4.92321360363797	-0.12962096661165	-0.45968124495553
H	-5.63042822425252	-0.15654928013269	0.36113670394706
C	-1.48626952470584	-0.06899776049977	3.41488161496273
H	-1.02574390381967	-0.06744568058401	4.40260196338571
C	-4.67681883832688	-0.09637459186400	-2.81523944708207
H	-5.22653987759121	-0.09930194287357	-3.75606656756022
C	-3.31950328402876	-0.06371096337593	-2.70174862386351
H	-2.69297078853273	-0.03777809188767	-3.59430342601458
C	-2.86040564083694	-0.11603006022022	3.36286986897193

H	-3.50021151218635	-0.14942612211773	4.24415938485105
N	3.55383481249992	0.12394055086432	2.19254742079130
N	-3.55365152688574	-0.12398417336104	2.19284310175792
N	-5.48363915424806	-0.12951514277617	-1.69561320031681
N	5.48350161294877	0.12940747985077	-1.69606752804514
O	4.80966586283097	0.16409476842755	2.22855164173056
O	-4.80947945347825	-0.16413986261155	2.22895108976716
O	-6.73060759862839	-0.15914793850236	-1.83470689198092
O	6.73045854940575	0.15903942106457	-1.83526449941451

2,2',10,10'-tetra-*N*-oxide-pBiphe (**45**), S_{0,eq} in methanol

N	1.34674537791574	0.01974868399482	-1.38876005255316
C	1.43984457720158	0.04897664413321	1.02196120140427
C	0.73752441154253	0.01709187485002	-0.23426256070800
C	3.53140133139044	0.09771526718753	-0.27671210775956
C	0.72661055388869	0.03284498465920	2.24413230730707
C	2.85388720213730	0.09806287474981	0.99465371023511
C	2.69512271454243	0.05324348611164	-1.43280822301765
C	4.92014675060300	0.13175175602911	-0.46261502106620
H	5.63018213344146	0.16648021027209	0.35549868739125
C	1.48280067494142	0.08335429692139	3.41481835426782
H	1.02381170215200	0.08442040910753	4.40322393936753
C	4.67526131286476	0.07742071361463	-2.81450200984187
H	5.22176715979419	0.07239977457073	-3.75750974803168
C	3.31735164528295	0.04483285784468	-2.70123527599733
H	2.69474560144783	0.01079878479992	-3.59625569507148
C	2.85707328041653	0.13743754537509	3.36100754604342
H	3.49265200536033	0.17885085167033	4.24546007101607
N	-1.34685818391097	-0.01985503678173	-1.38864768558040
C	-1.43975819049803	-0.04903825519481	1.02208118014675
C	-0.73754167977677	-0.01717657996608	-0.23420092811070
C	-3.53142222283982	-0.09780024837064	-0.27641857488950
C	-0.72642331967983	-0.03288347976049	2.24419304301946

C	-2.85380294966107	-0.09812681078691	0.99489134092489
C	-2.69523901012214	-0.05335015881848	-1.43258436970347
C	-4.92018288807801	-0.13183662489128	-0.46220701553478
H	-5.63015141442800	-0.16654749016504	0.35596544720633
C	-1.48251680390626	-0.08337236651810	3.41494233541703
H	-1.02344578962466	-0.08441896494354	4.40330984864030
C	-4.67549102667931	-0.07754889071460	-2.81411521961308
H	-5.22207428909804	-0.07254378652930	-3.75707819505984
C	-3.31757200952894	-0.04496153627914	-2.70096052989402
H	-2.69503882738834	-0.01094465800190	-3.59603233010349
C	-2.85679373063961	-0.13746080986825	3.36124616560261
H	-3.49229965455424	-0.17886062465301	4.24575155752163
N	3.54727725037923	0.14204426250384	2.19305066137932
N	-3.54709393345414	-0.14209054496837	2.19334613774303
N	-5.47490048335906	-0.12121565395260	-1.69520602200440
N	5.47476298845122	0.12111066768830	-1.69565946858896
O	4.81023534054599	0.18776356386276	2.23073226030401
O	-4.81004857085647	-0.18781499408316	2.23113196316375
O	-6.73321720040325	-0.15108558312344	-1.83248440775631
O	6.73306816418733	0.15098358842420	-1.83304231721582

2,2',10,10'-tetra-*N*-oxide-pBiphe (**45**), $S_{0,eq}$ in water

N	1.34865350173756	0.01472806192862	-1.39246611485468
C	1.43926577244312	0.05099950873440	1.01822813540925
C	0.73754727001323	0.01623662190239	-0.23816763804543
C	3.53163672842513	0.09877327316712	-0.27714451798020
C	0.72615503417646	0.03480240504707	2.24014234491100
C	2.85300623049693	0.10226998486203	0.99286240240753
C	2.69785860306861	0.04840565702162	-1.43401612702083
C	4.92055079645871	0.13405332681353	-0.45954201559688
H	5.62728574378195	0.17357556432499	0.36069242225921
C	1.48035975494173	0.08856231438741	3.41172475058730
H	1.01962798946187	0.08958714395652	4.39899291472267

C	4.68162250478912	0.06828718920821	-2.81079539405738
H	5.22900866575336	0.05941758515279	-3.75276924005196
C	3.32370741156470	0.03469934749449	-2.70037120973711
H	2.70579139732070	-0.00407871552131	-3.59781907200419
C	2.85407554293848	0.14596888770984	3.35931857777264
H	3.48799703656764	0.19030849004370	4.24428044853268
N	-1.34876659160154	-0.01483636996411	-1.39235365987123
C	-1.43917968551003	-0.05106195883059	1.01834819296236
C	-0.73756487099499	-0.01632294453594	-0.23810598618977
C	-3.53165765727333	-0.09885851870833	-0.27685085846947
C	-0.72596815085660	-0.03484131365817	2.24020315172814
C	-2.85292211863450	-0.10233454514256	0.99310012003951
C	-2.69797497687325	-0.04851353179921	-1.43379206866844
C	-4.92058673942368	-0.13413688027171	-0.45913387077665
H	-5.62725473331024	-0.17364030917398	0.36115919382088
C	-1.48007621257201	-0.08858021275585	3.41184874247361
H	-1.01926255149010	-0.08958501538796	4.39907871924617
C	-4.68185182131340	-0.06841496114370	-2.81040821237113
H	-5.22931522625422	-0.05956081123415	-3.75233731001075
C	-3.32392759366311	-0.03482905760062	-2.70009607849047
H	-2.70608454602729	0.00393086122819	-3.59759499025789
C	-2.85379618289159	-0.14599222228219	3.35955719005907
H	-3.48764493860038	-0.19031815546295	4.24457177569717
N	3.54534785938891	0.15031155168489	2.19194455332189
N	-3.54516463303247	-0.15035845337965	2.19224007271536
N	-5.47883572413409	-0.11858792947227	-1.69019036852805
N	5.47869864979826	0.11848484645659	-1.69064414114862
O	4.80968170671310	0.19933533861238	2.23174035268527
O	-4.80949480495914	-0.19938794030092	2.23214014140765
O	-6.73935826459404	-0.14974878644654	-1.82445845164232
O	6.73920982417041	0.14965067333591	-1.82501687698597

2,2',10,10'-tetra-*N*-oxide-pBiphe (**45**), T_{1,eq} in vacuum

N	1.34780059246168	0.03568783603948	-1.41622019812904
C	1.41809179194198	0.03767019403736	1.01744477095339
C	0.71576326328278	0.01896380162351	-0.22413468647172
C	3.51903617768537	0.09345551198001	-0.27582261810429
C	0.70776095016050	0.01881663072052	2.25136860448833
C	2.84156039808138	0.07551993939695	0.99276545600850
C	2.66203794753143	0.07060385023349	-1.44374392159208
C	4.90030910271495	0.13016098780222	-0.45252719849470
H	5.60928959480902	0.14906623954017	0.36798902785451
C	1.49002631251451	0.03969915070463	3.44128572809743
H	1.02455894042684	0.02739985533520	4.42610162940795
C	4.65726952831565	0.12351283169195	-2.82795874007409
H	5.22325193874160	0.13847752492494	-3.75883255315834
C	3.30944234426606	0.08771166618466	-2.72376031392382
H	2.67613012454536	0.07081585790509	-3.61097977944323
C	2.84305829439890	0.07570706111062	3.38223149968551
H	3.50901266866271	0.09349570113844	4.24354634833456
N	-1.34791508891682	-0.03579133910693	-1.41610845041318
C	-1.41800558423546	-0.03773221005993	1.01756237736264
C	-0.71577942626447	-0.01904694543841	-0.22407534544067
C	-3.51905658976349	-0.09354029974766	-0.27553074849765
C	-0.70757305923877	-0.01885721046039	2.25142731092496
C	-2.84147618737219	-0.07558280865299	0.99300113138159
C	-2.66215472141691	-0.07070813167989	-1.44352314437523
C	-4.90034410272706	-0.13024924247000	-0.45212073025794
H	-5.60925684237193	-0.14914089009187	0.36845433372161
C	-1.48974022054739	-0.03971924826548	3.44140932894955
H	-1.02419155293594	-0.02740275408479	4.42618660367395
C	-4.65750056936468	-0.12364091205440	-2.82757237354627
H	-5.22355981876687	-0.13862135679706	-3.75839921509070
C	-3.30966480326546	-0.08783762218088	-2.72348580248610
H	-2.67642584980892	-0.07095646394937	-3.61075785374821
C	-2.84277707619160	-0.07572856301342	3.38246732718939

H	-3.50866043974411	-0.09350239373788	4.24383735488691
N	3.53495508393434	0.09404028992738	2.18053559952828
N	-3.53477292106369	-0.09408289401949	2.18082879752776
N	-5.46367902680946	-0.14514281069825	-1.69470776600024
N	5.46354147936869	0.14503346196790	-1.69516101524278
O	4.79151149546024	0.12748613628458	2.23316494668947
O	-4.79132498677256	-0.12752828444809	2.23356230679657
O	-6.71040651994784	-0.17827746396791	-1.83554567324004
O	6.71025735822164	0.17816531637596	-1.83610235573260

2,2',10,10'-tetra-*N*-oxide-pBiphe (**45**), S_{1,eq} in vacuum

N	1.33024248723422	0.03524374604096	-1.39979729373339
C	1.43913414566015	0.03829643580166	1.02831247327879
C	0.73396023833748	0.01946783249371	-0.22725323144628
C	3.51365847282271	0.09337554528811	-0.27754045160102
C	0.71329135522771	0.01899841176202	2.25561528980707
C	2.84890951468443	0.07584472432583	0.99967977136443
C	2.67094453708410	0.07085627210363	-1.43753398611873
C	4.89993975612989	0.13014314112987	-0.45888382559495
H	5.59981675987666	0.14882249304963	0.37163706317119
C	1.50083380869695	0.04004343142278	3.43033387574174
H	1.04272951328802	0.02787015875926	4.41908360942521
C	4.64920022588676	0.12317503565767	-2.82946842704762
H	5.20973396919801	0.13792705016464	-3.76330114139905
C	3.29510792153029	0.08726970395195	-2.71322077294095
H	2.65570942000146	0.07019470021319	-3.59642242345411
C	2.86684508638661	0.07648604181830	3.36828387200145
H	3.52156765492856	0.09400277753051	4.23865047569073
N	-1.33035578385482	-0.03534739782984	-1.39968698728337
C	-1.43904705456207	-0.03835880361732	1.02843182466534
C	-0.73397680167687	-0.01955170610497	-0.22719239325765
C	-3.51367913030151	-0.09346029899613	-0.27724893853629
C	-0.71310298502060	-0.01903960224436	2.25567443032064

C	-2.84882476837975	-0.07590751777104	0.99991610158842
C	-2.67106093481706	-0.07096062355099	-1.43731236901054
C	-4.89997537145352	-0.13023111477457	-0.45847736989307
H	-5.59978381944122	-0.14889638419954	0.37210159080998
C	-1.50054855292701	-0.04006407723581	3.43045830005414
H	-1.04236267168574	-0.02787355447727	4.41917003344451
C	-4.64943135674827	-0.12330305916633	-2.82908275706538
H	-5.21004204570049	-0.13807089860074	-3.76286901514236
C	-3.29532950021601	-0.08739559690875	-2.71294737178524
H	-2.65600370629782	-0.07033541589888	-3.59620192170651
C	-2.86656495649567	-0.07650767961481	3.36852164267421
H	-3.52121572741435	-0.09400914488077	4.23894255526614
N	3.56496671567373	0.09504808587359	2.18796049085783
N	-3.56478392782014	-0.09509026934483	2.18825617688683
N	-5.45668171705885	-0.14483541483180	-1.70229243260700
N	5.45654349671307	0.14472627678571	-1.70274504701593
O	4.83064806867320	0.12884277048631	2.22474327357446
O	-4.83046223833718	-0.12888431177675	2.22514385294626
O	-6.69553701480480	-0.17766239988597	-1.84639162038093
O	6.69538691697974	0.17755063705212	-1.84694692654906

46, S_{0,eq} in vacuum

N	1.34475697655650	0.03447991188673	-1.43535729091038
C	1.43080412680227	0.04828946491617	0.98427785992401
C	0.73619865904977	0.02318813335473	-0.28211426875760
C	3.50084701281883	0.09974363290677	-0.30385513290759
C	0.75030972441141	0.03493669736960	2.21943681768106
C	2.84728562079790	0.08760588298570	0.95150886942105
C	2.70567373944260	0.07190671865512	-1.48276947280639
C	3.60732419858740	0.11450416861279	2.15200274460525
C	4.91989238781288	0.13876184439339	-0.38087462143418
C	1.52105357899440	0.06213212938720	3.39520887083079
H	1.02732824715225	0.05302143281041	4.36717740228475

C	4.73903853560989	0.12179273696471	-2.80439482091852
H	5.22705979721704	0.13049227055111	-3.78185043003576
C	3.35020548215421	0.08363163744807	-2.73162001850651
H	2.72538841418676	0.06192234386635	-3.62599042518684
C	5.51995698988020	0.14916015122492	-1.64858031639193
H	6.60982441502041	0.17900619244983	-1.72376190744440
C	2.90675088551695	0.10078582459916	3.36733070688374
H	3.46524095473355	0.12089994099699	4.30655853594509
N	-1.36307621834886	-0.03888533163916	-1.41438453657948
C	-1.43245816760184	-0.03147750218344	1.00277882850778
C	-0.74535405343687	-0.01748059419481	-0.26783563839450
C	-3.52798175379183	-0.09499780027631	-0.28165958106714
C	-0.71698571194934	-0.00634290761319	2.23503497148692
C	-2.85129108136064	-0.07118082043678	0.99553024774266
C	-2.72114301300575	-0.07674513904062	-1.45243176860880
C	-3.54008422447739	-0.08559638927531	2.22507269597047
H	-4.62959275481894	-0.11598479123327	2.24153423905896
C	-4.93014394504126	-0.13478240395681	-0.43051705796116
H	-5.57255206478384	-0.14956407236470	0.45118025648613
C	-1.44372775627678	-0.02204703111443	3.42248680393213
H	-0.92843599934801	-0.00382607769622	4.38278516535774
C	-4.70945029662231	-0.13721932564462	-2.84201250398404
H	-5.17833100692646	-0.15380340089079	-3.82854880083429
C	-3.33725253795119	-0.09849600640105	-2.72619419594280
H	-2.67811738657081	-0.08323665093737	-3.59583073663541
C	-5.51018061428073	-0.15548061731940	-1.68403561785141
H	-6.59826099194009	-0.18623201935498	-1.77619824601398
C	-2.84184051233712	-0.06134750811839	3.41552929748531
H	-3.38308367159660	-0.07278009525892	4.36424466495935
C	5.03645397188481	0.15381131365035	2.05677027114416
C	5.66390098976435	0.16538645779959	0.84615764834245
H	5.61935165285565	0.17443598219894	2.98100355785304
H	6.75509740121660	0.19541161592199	0.79210693327024

47, $S_{0,eq}$ in vacuum

N	1.36118444949011	0.03513249799956	-1.45003059338222
C	1.42821674995057	0.04808760818722	0.97236914148091
C	0.74341886035590	0.02333968773221	-0.30097711126778
C	3.50768376639979	0.10001145775290	-0.30140553334664
C	0.74121025755637	0.03447649976645	2.20700478660734
C	2.84477169973782	0.08737947254918	0.94932403983774
C	2.72173331930538	0.07265214915359	-1.48669846834151
C	3.59760204041163	0.11383721862383	2.15533213785963
C	4.92737263906098	0.13908621347765	-0.36843465919377
C	1.50518493166531	0.06115315742862	3.38766706503940
H	1.00413705396010	0.05162535073784	4.35603531468802
C	4.76460662132349	0.12313448290755	-2.79367516511228
H	5.26008049681564	0.13225921065149	-3.76736276618957
C	3.37563058268781	0.08491827482854	-2.73122263280421
H	2.75727460990303	0.06354279751700	-3.63006499939690
C	5.53665510790352	0.15002485355043	-1.63168281922982
H	6.62706820927247	0.17993074420872	-1.69856373657094
C	2.89069945706720	0.09970202346726	3.36714421907473
H	3.44470438726485	0.11942968465680	4.30903639896851
N	-1.36171471962504	-0.03952302786769	-1.44206818236087
C	-1.41516601928734	-0.03092041599463	0.98069321601703
C	-0.73751754520609	-0.01752893915973	-0.29664438139778
C	-3.50173631300718	-0.09409528495745	-0.28089142514868
C	-0.72124909463398	-0.00636699487112	2.21128646090191
C	-2.83182508980069	-0.07036706035569	0.96594004662487
C	-2.72244860624788	-0.07731585136297	-1.47076942738525
C	-3.57787797683454	-0.08608353680575	2.17634042641428
C	-4.92177847746298	-0.13370556625469	-0.33960985355484
C	-1.47858526477836	-0.02254465978284	3.39640663227314
H	-0.97213353537668	-0.00446611835402	4.36183515306052
C	-4.77262126873513	-0.13934396879096	-2.76577159297729

H	-5.27354208454572	-0.15710778187854	-3.73654869198150
C	-3.38331748853555	-0.10063000335653	-2.71144892415523
H	-2.77001141050504	-0.08727721743242	-3.61389835823585
C	-5.53813653618298	-0.15585989303351	-1.59927344521681
H	-6.62890849157970	-0.18631041029562	-1.65975534302016
C	-2.86419269631066	-0.06122583405232	3.38399470445307
H	-3.41290494378526	-0.07259037584419	4.32911719340939
C	5.02699784806404	0.15317055047411	2.06961965180407
C	5.66307611821716	0.16523941829689	0.86347296155691
H	5.60347232329354	0.17343803984023	2.99788971748308
H	6.75460267498563	0.19530881203993	0.81697900277158
C	-5.00772760091376	-0.12611735955379	2.09899608765760
C	-5.65055863614721	-0.14887348721029	0.89658830354101
H	-5.57900086046332	-0.13812025632118	3.03061859037130
H	-6.74232954472726	-0.17930616231203	0.85650685837387

48, S_{0,eq} in vacuum

N	1.35829682178320	-0.03532482559328	-1.39306561071600
C	1.45300279165627	0.00607850709717	1.02547597730559
C	0.75358776586797	-0.02347067000575	-0.24443647704083
C	3.54631248444542	0.01112293253911	-0.27450679641282
C	0.74130518477541	0.01696139447115	2.25390334660689
C	2.87036247856962	0.02378625907451	1.01182384871990
C	2.72131189073540	-0.01926259400321	-1.44970966917006
C	3.56257298421438	0.05251617758302	2.23426569553313
H	4.65261137696898	0.06636773529075	2.24678203120883
C	4.92721290290361	0.02644380134669	-0.42720513955103
H	5.57982177255477	0.04979828563964	0.44763162204114
C	1.47215745495692	0.04576522883549	3.44130739995368
H	0.96065216886288	0.05507981878672	4.40345857611701
C	4.70629649223417	-0.01801719745114	-2.86926199630635
C	3.31389391280657	-0.03318671784397	-2.71226714785127
H	2.64956997694304	-0.05631418349157	-3.57823080279211

C	5.53405102900501	0.01271961520141	-1.69574959211976
C	2.86770593976621	0.06333053809127	3.42988306863680
H	3.41293440382592	0.08572949271969	4.37607744978884
N	-1.33172048377548	-0.06649364674722	-1.40102598103913
C	-1.43391818258048	-0.03028977383771	1.01224163914551
C	-0.72915096020620	-0.04132109606052	-0.24672900245354
C	-3.51306499823381	-0.07636012326384	-0.29863953866209
C	-0.73164670095318	-0.00211818361442	2.24899370370908
C	-2.85324738487990	-0.04842235088613	0.98695645593402
C	-2.68960689422502	-0.08396268418273	-1.45776793551241
C	-3.55658476667999	-0.03849176925750	2.20764830765210
H	-4.64658984058863	-0.05215434751577	2.21178006300862
C	-4.91348286158943	-0.09618394318804	-0.46641141976945
H	-5.56806087137510	-0.09084462453311	0.40643800421291
C	-1.47232241575591	0.00658426697061	3.42726096270751
H	-0.97022934243639	0.02773131218656	4.39421734225106
C	-4.65924048685930	-0.12985485268158	-2.87428585053019
H	-5.11453499037990	-0.15062369795660	-3.86709601180724
C	-3.28830560669080	-0.11092597664545	-2.73968172231975
H	-2.61705710081468	-0.11583175632779	-3.60012244827417
C	-5.47632617173876	-0.12238917670548	-1.72763717545481
H	-6.56335563142407	-0.13738736724130	-1.83484376622911
C	-2.87099777587945	-0.01150482209489	3.40511385987057
H	-3.42220104102050	-0.00406031544612	4.34810486847646
C	6.94829796879916	0.02832179311519	-1.85589468151670
C	5.32958191047056	-0.03185640417029	-4.15027937932297
C	7.51404718230970	0.01429310724859	-3.10529792254337
C	6.69556732426362	-0.01615002647371	-4.26544854484758
H	7.57722977528268	0.05172231813325	-0.96207654907443
H	8.60103457088130	0.02652123633347	-3.21389174973660
H	7.16234367638579	-0.02700944758616	-5.25310393231169
H	4.69498226681840	-0.05526124585895	-5.03959737951413

49, $S_{0,eq}$ in vacuum

N	1.33436973085563	-0.03550213227493	-1.47363120525481
C	1.36348383331445	0.00383104039007	0.94647997799798
C	0.69835487002579	-0.02424633540355	-0.34163393168817
C	3.49112186553275	0.00827079740946	-0.29647165787623
C	0.61910857027841	0.01443056504151	2.15533280934402
C	2.78075683055623	0.02037652144133	0.97090235769869
C	2.69798700916663	-0.02035933635633	-1.49351869153814
C	3.44013480389457	0.04752103742745	2.21153467261703
H	4.52944707658445	0.06044071072504	2.25331770970512
C	4.87570459521065	0.02258328315992	-0.41192144994293
H	5.50446017248868	0.04456008855336	0.48023879250393
C	1.31798059879427	0.04158178501833	3.36175376503051
H	0.78131305712936	0.05050841829396	4.31000782734268
C	4.72053601502595	-0.01932354759208	-2.85912896378003
C	3.32452618308865	-0.03352862485661	-2.73984339381419
H	2.68382121456572	-0.05531451883153	-3.62345248539628
C	5.51640543226568	0.00958027604814	-1.66361341601654
C	2.71352947894809	0.05792107508494	3.38788430286146
H	3.23312690445437	0.07903251680570	4.34841568208657
N	-1.35115109580989	-0.06559513203499	-1.55334129052182
C	-1.52451711269704	-0.03033569125212	0.86078092114242
C	-0.78378467397360	-0.04131502967797	-0.38563381531842
C	-3.57427442446822	-0.07472453518549	-0.50604012595333
C	-0.85349664368897	-0.00324517655928	2.11163841870781
C	-2.94074134409553	-0.04736854198644	0.80124441968444
C	-2.71118363665451	-0.08250330826774	-1.65401183513971
C	-3.67293031698764	-0.03721638451916	2.00062349380381
H	-4.76280116511004	-0.05002245795733	1.97747862900931
C	-4.94949835969264	-0.09350644606243	-0.70341891346589
H	-5.63056447689045	-0.08818521515854	0.14974515885077
C	-1.62309450290028	0.00588322175815	3.27448214537186
H	-1.14375395282227	0.02644407635261	4.25282305460681

C	-4.64864496163724	-0.12743612704028	-3.13720515064246
C	-3.26225126445920	-0.10844727264332	-2.93530851585694
H	-2.56978057796727	-0.11349943067459	-3.77923083439369
C	-5.51438546386846	-0.11976788835273	-1.99092038409530
C	-3.01774105706572	-0.01097444727196	3.21794752270168
H	-3.59352694208177	-0.00326939739619	4.14610157397200
C	6.93450070583404	0.02415444285499	-1.78558269319175
C	5.37823540388450	-0.03241740914206	-4.12292259270321
C	7.53369799211278	0.01088266547887	-3.01926477320030
C	6.74679302995561	-0.01773226815268	-4.20116009086392
H	7.53911410138211	0.04615027959076	-0.87510483481190
H	8.62323245759300	0.02230822481056	-3.09845145618909
H	7.24005159875383	-0.02800326144412	-5.17586194785922
H	4.76786922964905	-0.05441883829255	-5.02907670638688
C	-5.22978755186109	-0.15410474488961	-4.43776669924332
C	-7.44727138011700	-0.16465039875510	-3.46372385826016
C	-6.92268375369043	-0.13912821692321	-2.19669297333163
H	-7.58056862292145	-0.13326160081883	-1.32368548423496
H	-8.53015669208447	-0.17931937193425	-3.60735164400293
H	-4.56645265948566	-0.15980098922887	-5.30616007526878
C	-6.59126236188827	-0.17222082817859	-4.59694207998645
H	-7.02555776642617	-0.19261612112965	-5.59915926480948

50, S_{0,eq} in vacuum

N	1.33379127426031	-0.03502462488823	-1.50858655149070
C	1.34851009653612	0.00300090830777	0.91232296591905
C	0.69048074180455	-0.02453533850949	-0.37886621147820
C	3.47090581269695	0.00760884394075	-0.30791398206107
C	0.62744835771118	0.01381441955633	2.11891633412031
C	2.76805475567368	0.01900752118031	0.92419570227720
C	2.69931881522899	-0.01993133841590	-1.51763744754378
C	3.48043656742055	0.04608520995642	2.15146768437416
C	4.88271130058408	0.02289316037823	-0.33794260288332

C	1.35673822624690	0.04074043823814	3.32711020491144
H	0.82725633372499	0.04964472973545	4.27977345191170
C	4.76914550915589	-0.01705424969803	-2.80948651387698
C	3.35957203879701	-0.03165795309808	-2.73631865134310
H	2.75546749095764	-0.05264904198348	-3.64525593408355
C	5.55395214777189	0.01053293156273	-1.61039220229041
C	2.73705230548948	0.05642873437921	3.34748447866026
H	3.26606861887793	0.07716389499146	4.30351208256846
N	-1.36796174914113	-0.06634608584311	-1.57724893360608
C	-1.52042402186670	-0.03020772933041	0.84045884676253
C	-0.79088749254151	-0.04166883065283	-0.41358482384840
C	-3.58112406228916	-0.07459083882843	-0.50944133935117
C	-0.84039267023005	-0.00297010148286	2.08932088077175
C	-2.93671219583146	-0.04681164004516	0.79259107987072
C	-2.72835343184114	-0.08310993390810	-1.66548231806329
C	-3.66022603777018	-0.03587594287526	1.99800173418672
H	-4.75020225368515	-0.04828457434474	1.98271230241360
C	-4.95808458343996	-0.09317869348308	-0.69496718784842
H	-5.63159660784587	-0.08731174213439	0.16412705350525
C	-1.60179166456535	0.00698392889818	3.25819585251731
H	-1.11404283682042	0.02780947134702	4.23248100605517
C	-4.67898559898879	-0.12838741056432	-3.13144665151265
C	-3.29105721861045	-0.10959264171447	-2.94201970869648
H	-2.60617700298154	-0.11518082591304	-3.79211303821393
C	-5.53438023577838	-0.11995031694892	-1.97732184636563
C	-2.99677700197228	-0.00932344898928	3.21090156048676
H	-3.56661773187257	-0.00095477145021	4.14273072500029
C	6.96440011484498	0.02439765453860	-1.73815425341332
C	5.42697724730686	-0.02943939830213	-4.06928313213099
C	7.57277752659892	0.01185474060131	-2.97355570909600
C	6.79769787200282	-0.01537726634002	-4.15362553123486
H	7.58841265170036	0.04545286993888	-0.84405933519118
H	8.66301845471122	0.02307170035855	-3.04085795379738

H	7.28992996499408	-0.02516088403503	-5.12869309605048
H	4.81420464905000	-0.05049464067574	-4.97376970506269
C	-5.27183393396835	-0.15557737101895	-4.42680389204602
C	-7.48039801936075	-0.16513521540268	-3.43272184653983
C	-6.94448852349364	-0.13909981482362	-2.17047289972265
H	-7.59450650553311	-0.13264290994950	-1.29160068961117
H	-8.56453357022967	-0.17963155892446	-3.56660240115125
H	-4.61632681565176	-0.16184931204740	-5.30111411184030
C	-6.63462965686608	-0.17346677206016	-4.57367860123529
H	-7.07797994365108	-0.19426645940450	-5.57190973443753
C	4.90382197666741	0.06119855335907	2.10528533874572
C	5.57295323727932	0.05005685132425	0.91233151471504
H	5.45998260330201	0.08199157488460	3.04568512258301
H	6.66320467543037	0.06230154060876	0.92322291476163

51, $S_{0,eq}$ in vacuum

N	1.35229037017829	-0.03530345686814	-1.53152507210471
C	1.34635562188742	0.00248447577543	0.89138059190672
C	0.69959916291575	-0.02505427065513	-0.40619015017860
C	3.47832370687391	0.00756151526218	-0.31213846348627
C	0.61636790101830	0.01316568426074	2.09581299019021
C	2.76535106874076	0.01870365330331	0.91450666313214
C	2.71706474446179	-0.01995348239110	-1.52856494272667
C	3.46878782557629	0.04577690449775	2.14772048701430
C	4.89043533253886	0.02308879552635	-0.33093000978975
C	1.33743811559591	0.04006192105978	3.30961900091899
H	0.79998284442853	0.04876479451882	4.25793858704355
C	4.79739484301038	-0.01652916516738	-2.80373944854139
C	3.38771405724446	-0.03138631082666	-2.74232388036424
H	2.79103897354437	-0.05234823361776	-3.65614816091619
C	5.57210279495852	0.01101403039284	-1.59790547562065
C	2.71733906700327	0.05590356159453	3.33896884282777
H	3.24037317875421	0.07659158327700	4.29829002945475

N	-1.36512758155020	-0.06727220055924	-1.61179152823644
C	-1.50309170307845	-0.03068735849764	0.80716928387668
C	-0.78042009358714	-0.04239321044858	-0.44991823117216
C	-3.55987615461847	-0.07463120566842	-0.52011154148892
C	-0.84590406226849	-0.00371475860481	2.05260290141602
C	-2.92098112510276	-0.04744989784379	0.74648099080560
C	-2.72767699846005	-0.08381611506889	-1.68943381722445
C	-3.69644647964110	-0.03723879419401	1.93596099078431
C	-4.96839445810255	-0.09199860269915	-0.62224901332800
C	-1.63783880449101	0.00603082129319	3.22167326639495
H	-1.15749918561740	0.02689675842771	4.20001013791380
C	-4.72856572137288	-0.12842508101814	-3.08524763974795
C	-3.32500773577880	-0.11033986626220	-2.94066148708476
H	-2.67496745022467	-0.11691994466100	-3.81755131897977
C	-5.57356907813924	-0.11953145652776	-1.92727209660752
C	-3.01706185328131	-0.01012034293767	3.16950058240448
H	-3.59615899203445	-0.00183322410589	4.09625621591022
C	6.98351620802631	0.02512194833392	-1.71394616564324
C	5.46590407025837	-0.02860801661581	-4.05808361529854
C	7.60228459263995	0.01286306858319	-2.94420809572395
C	6.83720917006838	-0.01430830016952	-4.13086253092058
H	7.60003783650738	0.04613358463057	-0.81468001725793
H	8.69304686049979	0.02425467637038	-3.00225172281133
H	7.33764509739986	-0.02385261091661	-5.10174264328940
H	4.86081726864263	-0.04961653128406	-4.96772748378123
C	-5.32128750808056	-0.15563894537526	-4.37688447978674
C	-7.52012543569026	-0.16479575749273	-3.39117391135446
C	-6.97556907843156	-0.13853496437410	-2.12651511023890
H	-7.64463814590886	-0.13239445346195	-1.26539792801355
H	-8.60551792160726	-0.17899809770397	-3.51355232963188
H	-4.66308739345409	-0.16205610249158	-5.24910247485872
C	-6.68585203247090	-0.17348943357981	-4.53058115811520
H	-7.12771855212838	-0.19434741476311	-5.52931085332953

C	4.89209999661323	0.06111166503104	2.11226228516203
C	5.57084606048563	0.05021518111434	0.92458712521650
H	5.44102273389614	0.08188339955954	3.05692324521576
H	6.66093832266289	0.06263266894549	0.94422602953071
C	-5.11518562240894	-0.05492273074493	1.81652822239993
C	-5.72219778019086	-0.08112896967199	0.59088748751658
H	-5.71912744397456	-0.04716040738035	2.72720832143063
H	-6.81153343473640	-0.09396097710892	0.54590851918698

52, S_{0,eq} in vacuum

N	1.38665718972440	0.08589130202580	-1.37925201774263
C	1.43575465128521	0.06552986359230	1.03175835521819
C	0.75568959638977	0.05333007557508	-0.22190144485842
C	3.49907570507390	0.14976045811650	-0.24679232289543
C	0.73326939586288	0.02921608176981	2.27334517159665
C	2.86019266417352	0.11587011345037	1.01309086323108
C	2.72623556515649	0.13285168042489	-1.38761088059025
C	3.57222774489322	0.12984694640438	2.23769880693528
H	4.66373991503791	0.16846480280504	2.21961684730660
C	1.47679286767013	0.04491748549454	3.44474957581307
H	0.97634986690010	0.01851310526914	4.41301515808513
C	2.88363566487378	0.09482229584637	3.42707773063351
H	3.42635523036752	0.10543414708964	4.37508075245391
N	-1.32165369677482	-0.00706832008513	-1.39249466001005
C	-1.43244999227620	-0.03552172205730	1.02242597279424
C	-0.72377292924294	0.00196675183892	-0.23612274784441
C	-3.50602294335330	-0.09563584086743	-0.29813808199652
C	-0.73714352002366	-0.02300941381318	2.26432538330964
C	-2.85070497161768	-0.08538522848040	0.99110576151896
C	-2.67964203343954	-0.05430137444654	-1.45407567967604
C	-3.55812210726963	-0.12242813126491	2.20851647883397
H	-4.64756295632975	-0.16084767553631	2.20729095213927
C	-4.90479977556715	-0.14371126246034	-0.47100398325445

H	-5.56181422261154	-0.17626957477364	0.39944297408769
C	-1.48179510451996	-0.06106007610396	3.43996614921123
H	-0.98158907902882	-0.05294447994323	4.40848049231706
C	-4.64371866787044	-0.10910696808279	-2.87783841131161
H	-5.09537195943182	-0.11467616436724	-3.87251594152265
C	-3.27362982495773	-0.06189374163355	-2.73792280198209
H	-2.59999310128854	-0.02901778707100	-3.59589798430351
C	-5.46377145165860	-0.15035738534222	-1.73454501758039
H	-6.54987758842978	-0.18792719968452	-1.84556274230878
C	-2.87876152550823	-0.11029109279262	3.41060238540096
H	-3.43475373744012	-0.13923300035840	4.35036707639109
H	3.19897481965897	0.15823518004631	-2.37577984877172
H	4.58900031157247	0.18863614941561	-0.30780232062861

53, S_{0,eq} in vacuum

N	1.36186722201721	0.05911781621566	-1.38160335284801
C	1.42646917427254	0.06261417361492	1.03067195537982
C	0.73851433047279	0.03223302034786	-0.22045559192513
C	3.48083320193664	0.15238460516559	-0.26315503328165
C	0.73444233979930	0.03242996880663	2.27920682418802
C	2.84998971512081	0.12515646397375	1.00182304306788
C	2.70160243288236	0.11772485109292	-1.39854231093455
C	3.57029100744937	0.15725516051251	2.22092591101703
H	4.66128466445320	0.20520485622382	2.19424363674846
C	1.48601092065835	0.06601220862497	3.44559452551201
H	0.99092298232550	0.04466673553250	4.41702501301387
C	2.89143954689287	0.12788957828283	3.41670402275574
H	3.44187129334687	0.15249778485496	4.35998841070275
N	-1.36196367066557	-0.05907164966332	-1.38150192881410
C	-1.42638385207942	-0.06261687399603	1.03077818401463
C	-0.73852327937703	-0.03221038112620	-0.22040059048658
C	-3.48084533451229	-0.15236099379464	-0.26289589400839
C	-0.73426297563479	-0.03245805906250	2.27926147862571

C	-2.84990652199204	-0.12515850958933	1.00203518462774
C	-2.70170015329536	-0.11767829810188	-1.39834118825376
C	-3.57011591863128	-0.15728194581743	2.22119164960416
H	-4.66111159003571	-0.20523102164768	2.19459111199813
C	-1.48574361717084	-0.06606397939025	3.44570522844066
H	-0.99058238674700	-0.04473834809439	4.41709879669485
C	-2.89117437041313	-0.12794072583454	3.41691927382310
H	-3.44153547974432	-0.15256814660448	4.36024437066295
H	-4.57000713914919	-0.20015577683256	-0.33086473421221
H	-3.16800108869814	-0.13762434738525	-2.38965349896610
H	3.16782867389652	0.13769100691029	-2.38988935522344
H	4.56998987262176	0.20018082678131	-0.33120514192362