Electronic Supplementary Information

Basically, nucleophilicity matters little: towards unravelling the supramolecular driving forces in enzyme-like CO_2 conversion

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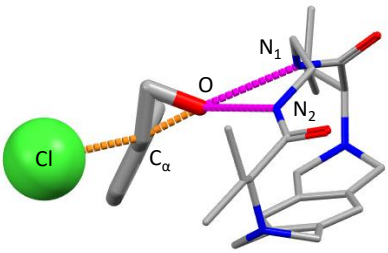
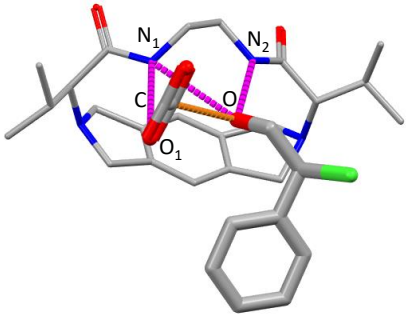
TS1



$Cl - C_\alpha = 2.76$; $O - N_1 = 2.98$
$O - C_\alpha = 1.78$; $O - N_2 = 2.85$

-253.2 *i* cm^{-1}

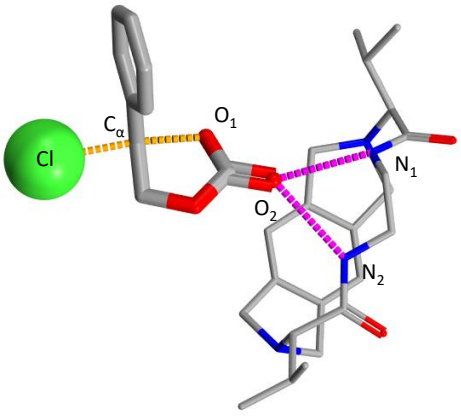
TS2



$O - C = 2.69$; $O_1 - N_1 = 3.36$
$O - N_1 = 3.26$; $O - N_2 = 2.69$

-23.9 *i* cm^{-1}

TS3



$Cl - C_\alpha = 2.56$; $O_2 - N_1 = 2.88$
$O_1 - C_\alpha = 1.94$; $O_2 - N_2 = 2.89$

-282.8 *i* cm^{-1}

Fig. S1. DFT (B3LYP) optimized structures for the transition states **TS1–TS3** together with the most relevant calculated distances (magenta discontinuous lines for hydrogen bonding and orange discontinuous lines for characteristic bond formation/breaking of each TS). The values of the negative (imaginary) vibrational frequencies have also been included.

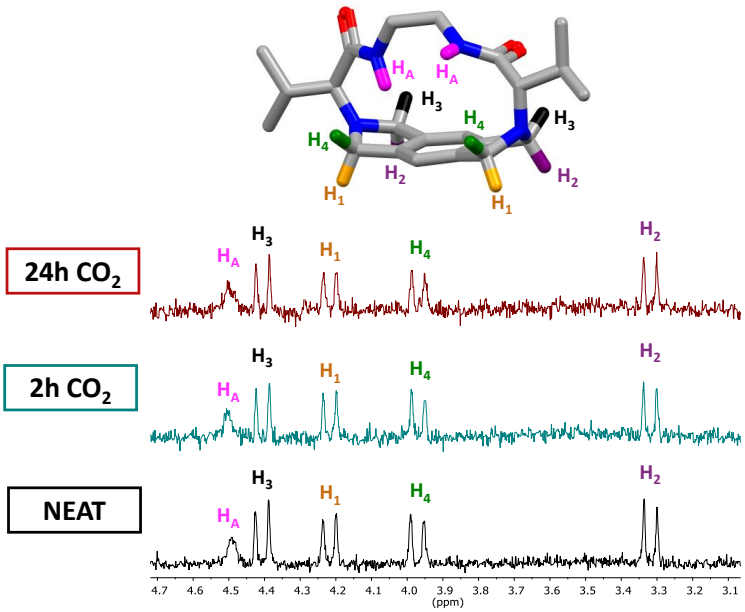


Fig. S2. Time evolution of the ^{1}H NMR (500 MHz, benzene-d_6, 25 ºC) partial spectra of macrocycle **1** in the presence of CO_2 (10 bar). The 4.7 – 3.1 region has been selected as it contains the signals for the diastereotopic isoindolinic protons adjacent to the tertiary amino groups. The relevant hydrogen atoms have been highlighted with different colours.

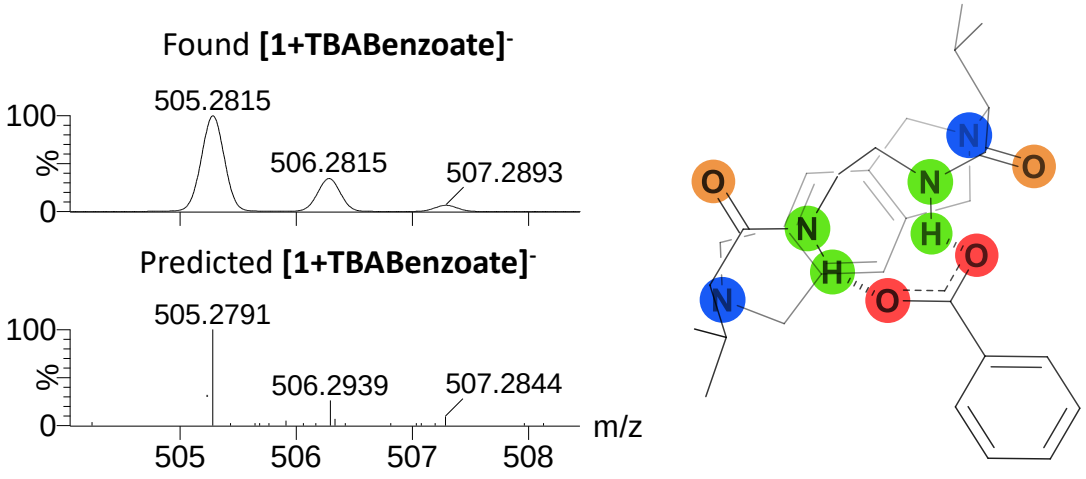


Fig. S3. HRMS (ESI-) analysis of a 1:10 mixture **1** : **TBABenzoate** in methanol. Below: predicted mass spectrum for the supramolecular complex. Above: experimental mass spectrum.

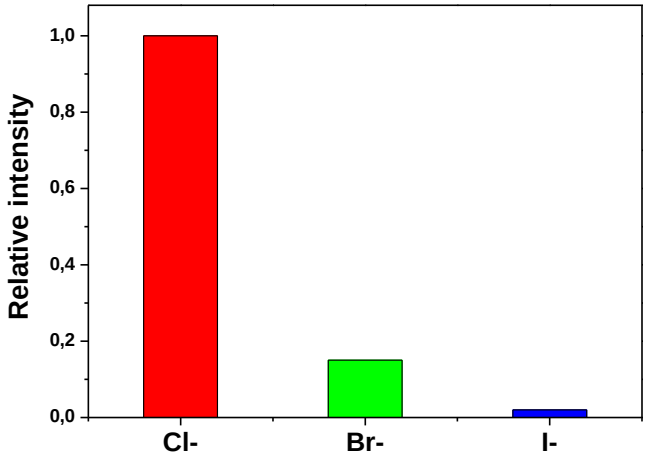


Fig. S4. HRMS-ESI (-) relative intensities of the peaks obtained for the competitive studies involving the formation of the supramolecular adducts **[1·X⁻]**. Relative intensities measured as follows: R= I_{X^-} / I_{Cl^-} , where X = Cl, Br, or I. Competition experiment conditions: equimolar mixture of **1** : **TBACl** : **TBABr** : **TBAI** (1 mM each) in benzene.

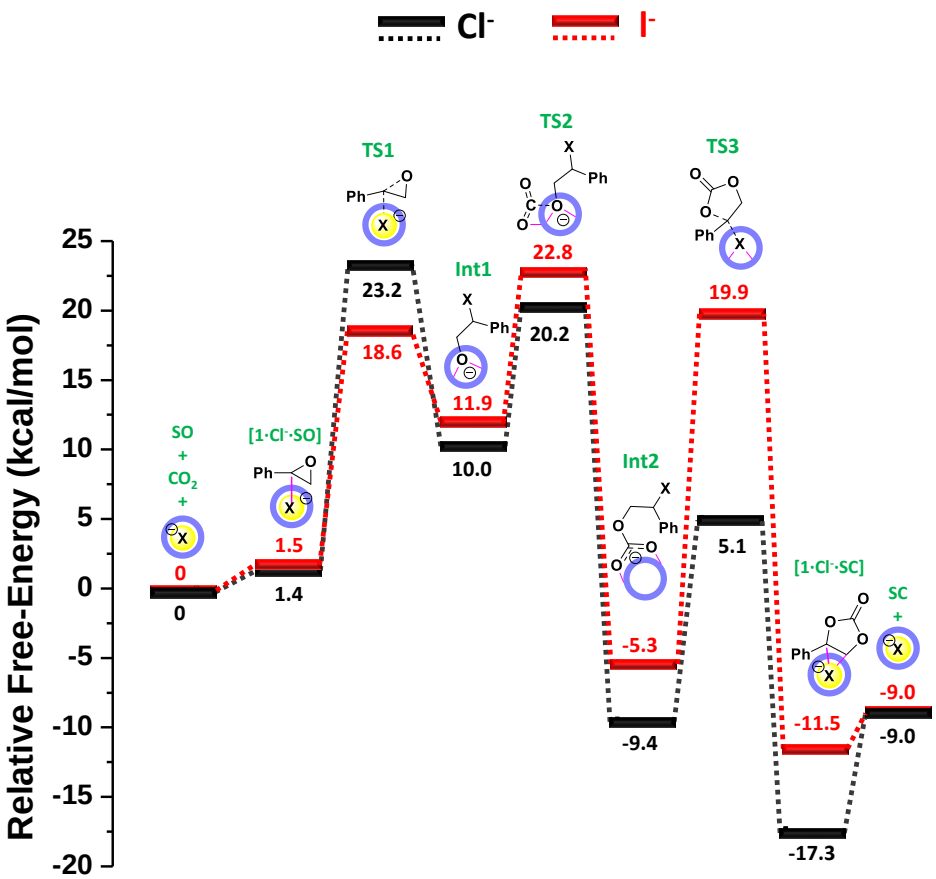


Fig. S5. Free-energy profiles for the cycloaddition of CO_2 to **SO** catalysed by **1** in the presence of chloride (black profile) and iodide (red profile) anion. The halide anion has been represented with a yellow sphere, and the macrocyclic scaffold with a blue circle. Hydrogen bonds have been highlighted with discontinuous magenta lines

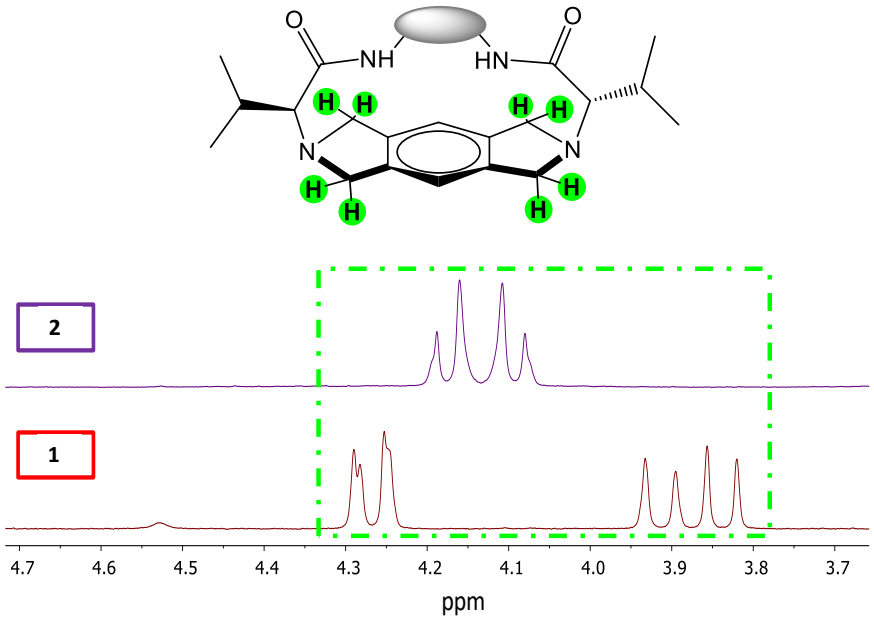


Fig. S6. Partial ^{1}H NMR (400 MHz, CD_3OD, 25 ºC) spectra (signals for the isoindolinic protons, highlighted in green) of the macrocyclic pseudopeptides **1** and **2**. Concentration: 6 mM.

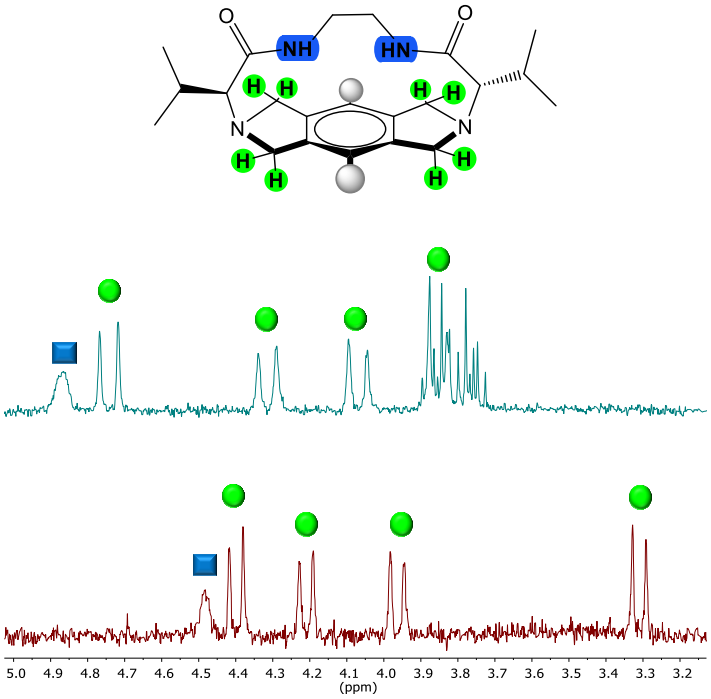


Fig. S7. Partial ^{1}H NMR (400 MHz, 2 mM in benzene-d_6, 25 ºC) spectra for the isoindolinic and amide group protons, highlighted in green and blue, respectively. Blue spectrum for **3** and red spectrum for **1**.

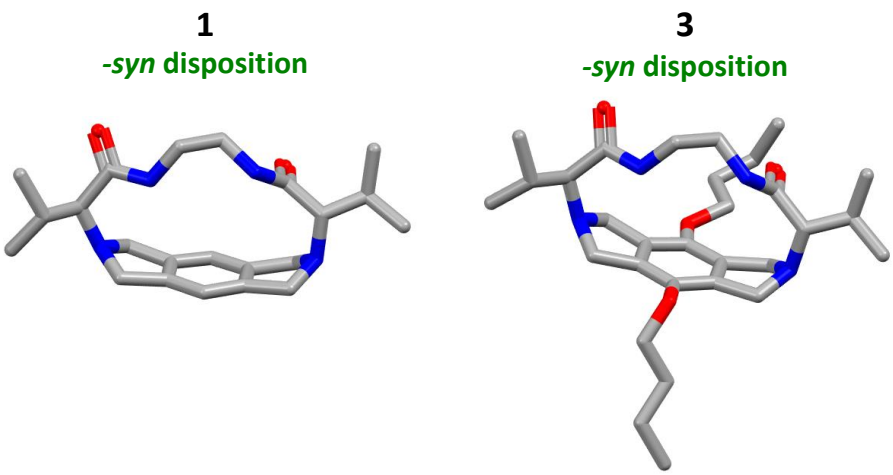


Fig. S8. DFT (B3LYP) optimized structures for the pseudopeptidic macrocycles **1** and **3**, both displaying *-syn* disposition for the amide groups.

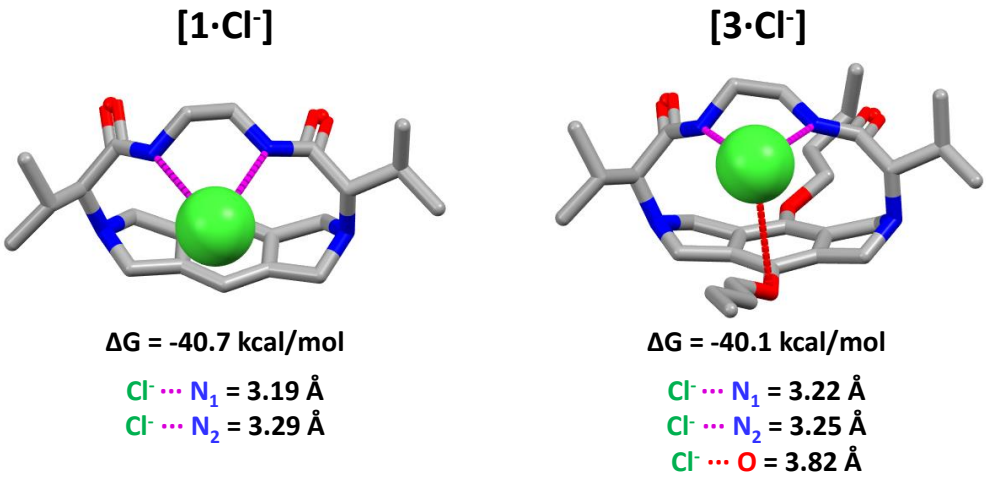


Fig. S9. DFT (B3LYP) optimized structures for the supramolecular complexes **[1·Cl$^-$]** and **[3·Cl$^-$]**. The free-energies of formation have been included, as well as the most relevant distances: stabilizing hydrogen bonding (discontinuous magenta lines) and repulsive polar interactions (discontinuous red lines).

DFT calculation details

- Lowest energy conformation for **Cl^-**.

Cartesian coordinates (1 atom), E (298.15 K) = -15.013656 Hartree

1	Cl	-2.1823	1.7893	0

- Lowest energy conformation for **Br^-**.

Cartesian coordinates (1 atom), E (298.15 K) = -13.253291 Hartree

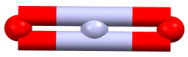
1	Br	1.1838	-0.9904	2.8477

- Lowest energy conformation for **I^-**.

Cartesian coordinates (1 atom), E (298.15 K) = -11.488958 Hartree

1	I	1.1838	-0.9904	2.8477

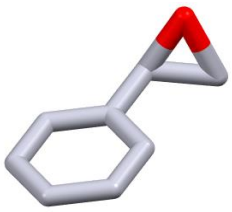
- Lowest energy conformation for CO_2



Cartesian coordinates (3 atoms). E (298.15 K) = -188.549993 Hartree

1	C	4.3494	3.3158	-0.1139
2	O	5.6078	3.3158	-0.1139
3	O	3.091	3.3158	-0.1139

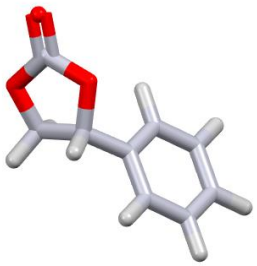
- Lowest energy conformation for **SO**



Cartesian coordinates (17 atoms). E (298.15 K) = -384.674236 Hartree

1	C	-3.1287	0.2627	0.0542
2	C	-1.7335	0.2627	0.0542
3	C	-1.036	1.4704	0.0542
4	C	-1.7336	2.6789	0.053
5	C	-3.1285	2.6789	0.0525
6	C	-3.8261	1.4707	0.0535
7	H	-3.6784	-0.6896	0.0547
8	H	-1.184	-0.6898	0.0555
9	H	0.0637	1.4705	0.0549
10	H	-3.6786	3.6311	0.0516
11	H	-4.9257	1.4708	0.0534
12	O	0.0424	4.3695	1.1823
13	C	-0.9631	4.0123	0.0529
14	H	-1.8223	4.529	-0.321
15	C	0.5285	3.9502	-0.3249
16	H	0.4734	4.2162	-1.3599
17	H	1.4644	3.4699	-0.1295

- Lowest energy conformation for **SC**

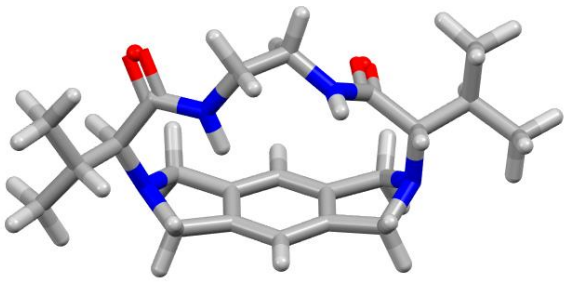


Cartesian coordinates (20 atoms). E (298.15 K) = -573.23857 Hartree

1	C	-3.0682	0.8196	-0.6341
2	C	-1.6633	0.7593	-0.6966
3	C	-0.8809	1.8007	-0.1588
4	C	-1.5172	2.9176	0.4267
5	C	-2.9197	2.9834	0.4787
6	C	-3.6992	1.9315	-0.0465
7	H	-3.6636	0.0099	-1.0471
8	H	-1.1798	-0.0959	-1.1656
9	H	-0.9206	3.7418	0.8076
10	H	-3.4046	3.8497	0.9177
11	H	-4.7841	1.9826	-0.004
12	C	0.6229	1.6869	-0.182
13	H	0.9411	0.9214	-0.8971

14	O	1.2545	2.968	-0.6131
15	O	2.537	2.2427	1.1333
16	C	2.428	3.1974	0.1155
17	O	3.2299	4.0883	-0.097
18	C	1.2872	1.4555	1.206
19	H	1.5538	0.4122	1.3847
20	H	0.6804	1.8435	2.028

- Lowest energy conformation for **1**.

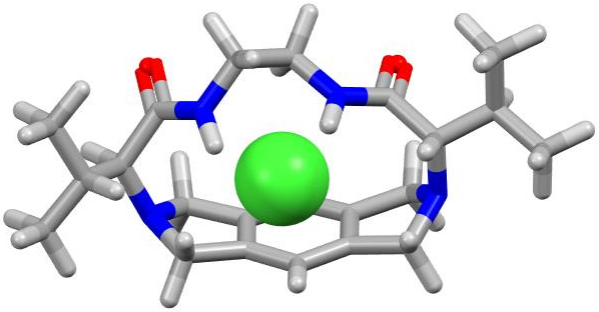


Cartesian coordinates (60 atoms), E (298.15 K) = -1226.405178 Hartree

1	H	-0.3201	1.1987	2.8274
2	C	-0.6832	1.3629	1.8145
3	C	-1.6241	1.7712	-0.8643
4	C	-1.8921	0.8075	1.3731
5	C	0.0823	2.0759	0.8743
6	C	-0.3711	2.2545	-0.4504
7	C	-2.3693	1.0269	0.061
8	H	-1.9662	1.8965	-1.8887
9	C	1.4957	2.6363	1.0043
10	H	1.4878	3.6092	1.5231
11	H	2.1634	1.9792	1.5744
12	C	0.7385	2.8856	-1.2835
13	H	0.5118	3.9346	-1.5338
14	C	-2.8258	-0.1876	2.0578
15	H	-2.3091	-0.9204	2.6879
16	H	-3.564	0.3281	2.6912
17	C	-3.653	0.217	-0.1284
18	H	-3.7536	-0.2134	-1.1262
19	H	-4.5409	0.8305	0.0843
20	N	-3.5452	-0.8536	0.9227
21	C	-2.9592	-2.1581	0.4657
22	H	-2.5114	-2.6244	1.357
23	C	-1.858	-2.0036	-0.6239
24	N	-0.5454	-2.1363	-0.2228
25	C	0.5714	-2.1155	-1.1899
26	H	0.7274	-3.1313	-1.5858
27	H	0.2701	-1.4854	-2.0308
28	C	1.9033	-1.6242	-0.5876
29	H	2.7157	-1.9418	-1.2483
30	H	2.0685	-2.0993	0.3933
31	N	2.0365	-0.1668	-0.4519
32	C	2.9582	0.5454	-1.198
33	C	3.1236	2.0771	-0.925
34	H	3.3438	2.4912	-1.9187
35	N	1.941	2.7894	-0.4088
36	H	0.8981	2.3518	-2.2302

37	C	4.3928	2.3657	-0.0459
38	H	4.2075	1.969	0.9651
39	C	5.6733	1.688	-0.586
40	H	6.5277	1.9711	0.0436
41	H	5.599	0.5971	-0.6001
42	H	5.8836	2.0107	-1.6138
43	C	4.6168	3.8926	0.0661
44	H	4.8497	4.3176	-0.9206
45	H	3.7308	4.4073	0.4493
46	H	5.4652	4.1038	0.7305
47	C	-4.0731	-3.118	-0.0501
48	H	-4.5326	-2.6377	-0.9258
49	C	-3.4821	-4.4751	-0.5007
50	H	-2.783	-4.3613	-1.3369
51	H	-2.9591	-4.9732	0.33
52	H	-4.2865	-5.1453	-0.83
53	C	-5.1541	-3.331	1.03
54	H	-5.5396	-2.3709	1.3859
55	H	-5.9876	-3.9209	0.6261
56	H	-4.7457	-3.8793	1.8927
57	O	-2.1538	-1.7659	-1.8285
58	O	3.6806	-0.0207	-2.0643
59	H	-0.3474	-2.3913	0.7383
60	H	1.3674	0.3269	0.1271

- Lowest energy conformation for **[1·Cl⁻]**.

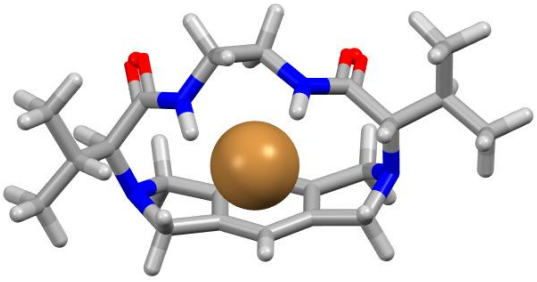


Cartesian coordinates (61 atoms), E (298.15 K) = -1241.483633 Hartree

1	H	-0.546	1.3861	2.7269
2	C	-0.8705	1.57	1.7084
3	C	-1.5963	1.8349	-1.0541
4	C	-2.0374	0.9919	1.2036
5	C	-0.0432	2.2417	0.7975
6	C	-0.3968	2.3836	-0.557
7	C	-2.3964	1.1074	-0.1577
8	H	-1.8453	1.8918	-2.1119
9	C	1.3791	2.7143	1.0209
10	H	1.4165	3.6485	1.6071
11	H	1.9471	1.9601	1.5778
12	C	0.7593	3.043	-1.3029
13	H	0.539	4.0989	-1.5341
14	C	-2.9734	-0.0021	1.8743
15	H	-2.4601	-0.6479	2.5935
16	H	-3.7988	0.5058	2.4005
17	C	-3.6032	0.1946	-0.4051
18	H	-3.5838	-0.3154	-1.3707
19	H	-4.5487	0.7545	-0.3247
20	N	-3.5421	-0.7945	0.7315
21	C	-2.8146	-2.0913	0.4633
22	H	-2.2404	-2.3263	1.3703
23	C	-1.8202	-2.0155	-0.7254
24	N	-0.5034	-1.8315	-0.4429
25	C	0.4629	-1.7256	-1.5515
26	H	0.3773	-2.6265	-2.1762
27	H	0.2027	-0.8761	-2.1958
28	C	1.9154	-1.5804	-1.0597
29	H	2.5768	-1.7997	-1.9042
30	H	2.1066	-2.2857	-0.2435
31	N	2.2495	-0.2361	-0.5632
32	C	2.7084	0.7305	-1.408
33	C	3.0682	2.1416	-0.8472
34	H	3.443	2.6579	-1.7427
35	N	1.9199	2.9475	-0.3551
36	H	0.99	2.5406	-2.2508

37	C	4.2517	2.0859	0.1629
38	H	3.9359	1.5276	1.056
39	C	5.4545	1.3322	-0.4532
40	H	6.2915	1.3091	0.2583
41	H	5.1973	0.2981	-0.7087
42	H	5.7978	1.8298	-1.3712
43	C	4.6772	3.5073	0.5964
44	H	5.0297	4.0829	-0.272
45	H	3.8423	4.0574	1.0408
46	H	5.497	3.457	1.3273
47	C	-3.8286	-3.2497	0.2268
48	H	-4.388	-3.0009	-0.6863
49	C	-3.1009	-4.5959	-0.0032
50	H	-2.4746	-4.5614	-0.901
51	H	-2.4626	-4.8485	0.857
52	H	-3.8305	-5.4088	-0.1282
53	C	-4.8164	-3.365	1.407
54	H	-5.2935	-2.398	1.5966
55	H	-5.5939	-4.1125	1.1911
56	H	-4.2956	-3.6793	2.3251
57	O	-2.2407	-2.1293	-1.925
58	O	2.8706	0.5156	-2.654
59	H	-0.1568	-1.6576	0.5176
60	H	2.0529	-0.0999	0.439
61	C	1.1427	-1.0868	2.309

- Lowest energy conformation for **[1·Br⁻]**.

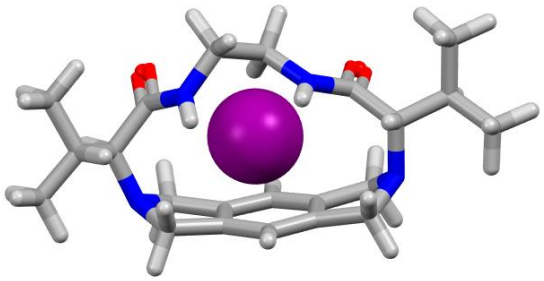


Cartesian coordinates (61 atoms), E (298.15 K) = -1239.707715 Hartree

1	H	-0.4964	1.3649	2.7267
2	C	-0.8299	1.5497	1.7109
3	C	-1.5855	1.827	-1.043
4	C	-1.9952	0.9609	1.2121
5	C	-0.0206	2.2401	0.7976
6	C	-0.3879	2.3852	-0.5536
7	C	-2.3705	1.0859	-0.1437
8	H	-1.8476	1.8923	-2.0971
9	C	1.3886	2.7576	1.0127
10	H	1.394	3.7041	1.5796
11	H	1.9873	2.0388	1.5835
12	C	0.7493	3.0761	-1.3016
13	H	0.5091	4.1323	-1.5088
14	C	-2.923	-0.0366	1.889
15	H	-2.3983	-0.6925	2.5909
16	H	-3.7329	0.4708	2.4389
17	C	-3.5841	0.1805	-0.3833
18	H	-3.5751	-0.3264	-1.3509
19	H	-4.5246	0.7475	-0.2954
20	N	-3.5202	-0.812	0.7495
21	C	-2.8279	-2.1218	0.4624
22	H	-2.2754	-2.3922	1.3731
23	C	-1.8139	-2.0413	-0.7096
24	N	-0.499	-1.8675	-0.4042
25	C	0.4872	-1.7451	-1.4937
26	H	0.4293	-2.6479	-2.1188
27	H	0.2225	-0.9017	-2.1428
28	C	1.9288	-1.5759	-0.9783
29	H	2.6053	-1.8165	-1.8052
30	H	2.1133	-2.2562	-0.1395
31	N	2.254	-0.217	-0.5157
32	C	2.6741	0.742	-1.3917
33	C	3.0556	2.1598	-0.864
34	H	3.4168	2.657	-1.7753
35	N	1.9223	2.9859	-0.3675
36	H	0.9793	2.5958	-2.2606
37	C	4.2572	2.1128	0.1252

38	H	3.9585	1.5656	1.0311
39	C	5.446	1.3489	-0.5054
40	H	6.2951	1.3287	0.1913
41	H	5.1815	0.3131	-0.7468
42	H	5.7751	1.8374	-1.4335
43	C	4.694	3.5375	0.5351
44	H	5.0287	4.1043	-0.346
45	H	3.8699	4.0936	0.992
46	H	5.5291	3.4922	1.2488
47	C	-3.8691	-3.2464	0.1859
48	H	-4.4109	-2.9628	-0.7277
49	C	-3.1751	-4.6064	-0.0661
50	H	-2.5344	-4.5686	-0.9536
51	H	-2.5581	-4.8978	0.7973
52	H	-3.925	-5.395	-0.2218
53	C	-4.8735	-3.3614	1.352
54	H	-5.3267	-2.3867	1.5593
55	H	-5.6679	-4.0827	1.1106
56	H	-4.3716	-3.71	2.2681
57	O	-2.2122	-2.1318	-1.9172
58	O	2.7819	0.508	-2.6387
59	H	-0.1751	-1.7327	0.564
60	H	2.117	-0.0568	0.4879
61	Br	1.2567	-1.2064	2.6258

- Lowest energy conformation for **[1·I⁻]**.

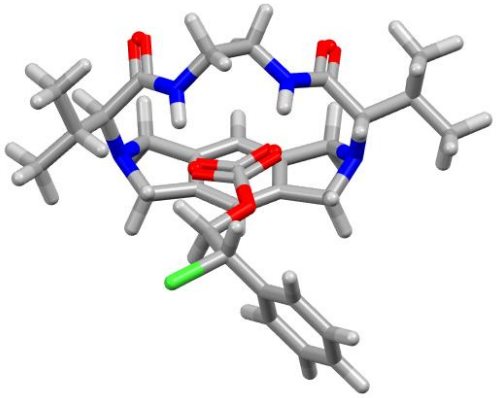


Cartesian coordinates (61 atoms), E (298.15 K) = -1237.929922 Hartree

1	H	-0.4692	1.366	2.735
2	C	-0.8047	1.5421	1.7178
3	C	-1.5825	1.828	-1.029
4	C	-1.9689	0.9451	1.2239
5	C	-0.0058	2.2414	0.8016
6	C	-0.3843	2.3899	-0.5466
7	C	-2.3564	1.0777	-0.1277
8	H	-1.8557	1.9011	-2.0798
9	C	1.3959	2.785	1.0083
10	H	1.3839	3.7377	1.5639
11	H	2.014	2.0879	1.5849
12	C	0.7386	3.102	-1.2969
13	H	0.4861	4.1591	-1.4832
14	C	-2.8932	-0.0539	1.9044
15	H	-2.365	-0.7178	2.5964
16	H	-3.6928	0.4543	2.4683
17	C	-3.5766	0.1799	-0.3608
18	H	-3.5785	-0.3221	-1.3309
19	H	-4.5125	0.7528	-0.2626
20	N	-3.5086	-0.8174	0.7669
21	C	-2.8367	-2.1332	0.4641
22	H	-2.2988	-2.4282	1.3761
23	C	-1.811	-2.0463	-0.6972
24	N	-0.4944	-1.8952	-0.3788
25	C	0.5018	-1.7602	-1.4582
26	H	0.4604	-2.6627	-2.0852
27	H	0.2316	-0.9199	-2.1078
28	C	1.938	-1.5765	-0.9338
29	H	2.6197	-1.8285	-1.7536
30	H	2.1247	-2.2454	-0.086
31	N	2.2608	-0.2106	-0.4899
32	C	2.6366	0.7498	-1.3868
33	C	3.0412	2.1682	-0.8795
34	H	3.3911	2.6532	-1.8015
35	N	1.922	3.0107	-0.3756
36	H	0.9642	2.6394	-2.2652

37	C	4.2578	2.1218	0.091
38	H	3.9717	1.5863	1.0082
39	C	5.4305	1.343	-0.5518
40	H	6.2911	1.3245	0.1305
41	H	5.1561	0.306	-0.7766
42	H	5.7471	1.8196	-1.4904
43	C	4.7111	3.5471	0.4802
44	H	5.0373	4.1028	-0.4111
45	H	3.8979	4.1138	0.9435
46	H	5.5558	3.5019	1.1822
47	C	-3.8929	-3.2359	0.1582
48	H	-4.423	-2.9274	-0.7544
49	C	-3.2181	-4.6018	-0.1136
50	H	-2.5662	-4.5576	-0.9925
51	H	-2.6172	-4.9215	0.751
52	H	-3.9792	-5.374	-0.2945
53	C	-4.9082	-3.3564	1.3141
54	H	-5.35	-2.3795	1.5349
55	H	-5.7101	-4.0626	1.054
56	H	-4.4186	-3.7273	2.228
57	O	-2.1971	-2.1054	-1.9093
58	O	2.6819	0.5113	-2.6356
59	H	-0.1812	-1.8052	0.5935
60	H	2.1897	-0.0405	0.5157
61	I	1.419	-1.3362	2.9499

- Lowest energy conformation for **[1·Int2]**.

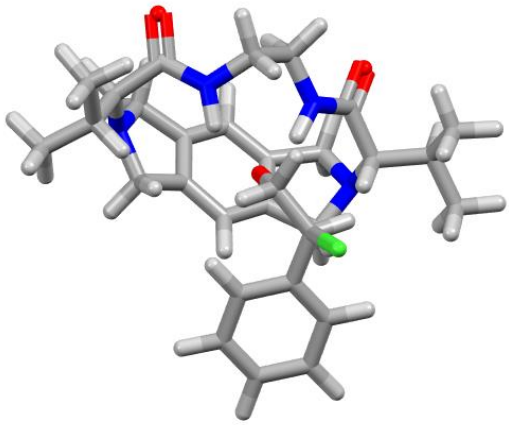


Cartesian coordinates (81 atoms), E (298.15 K) = -2279.366513 Hartree

1	H	0.0281	1.122	3.0273
2	C	-0.4438	1.3097	2.0665
3	C	-1.611	1.6842	-0.5221
4	C	-1.645	0.6856	1.7152
5	C	0.1941	2.0832	1.0865
6	C	-0.3749	2.2696	-0.1885
7	C	-2.2269	0.8685	0.4417
8	H	-2.0333	1.7906	-1.5193
9	C	1.5856	2.6885	1.1231
10	H	1.5992	3.6305	1.6976
11	H	2.3015	2.0068	1.5903
12	C	0.6111	3.0474	-1.0577
13	H	0.3013	4.0999	-1.1686
14	C	-2.4284	-0.3819	2.4669
15	H	-1.7783	-1.0716	3.0144
16	H	-3.1353	0.0661	3.1852
17	C	-3.446	-0.0536	0.3376
18	H	-3.5657	-0.5147	-0.6458
19	H	-4.3727	0.4892	0.584
20	N	-3.2	-1.0955	1.3957
21	C	-2.5775	-2.3874	0.9306
22	H	-1.9272	-2.7315	1.7459
23	C	-1.7052	-2.2179	-0.3438
24	N	-0.3703	-2.0361	-0.1677
25	C	0.4928	-1.8241	-1.3425
26	H	0.4156	-2.7035	-1.9995
27	H	0.1308	-0.9728	-1.9298
28	C	1.9734	-1.6063	-0.9707
29	H	2.5671	-1.8363	-1.8636
30	H	2.2636	-2.2917	-0.1658
31	N	2.3193	-0.242	-0.5388
32	C	2.5215	0.7413	-1.4608
33	C	2.9671	2.1584	-0.9839
34	H	3.1798	2.6716	-1.9323

35	N	1.9125	2.9698	-0.3113
36	H	0.7161	2.6229	-2.0632
37	C	4.3027	2.1149	-0.184
38	H	4.1503	1.5403	0.7407
39	C	5.3964	1.3906	-1.0047
40	H	6.3374	1.3604	-0.4384
41	H	5.11	0.3593	-1.2405
42	H	5.5845	1.9138	-1.9533
43	C	4.773	3.5385	0.1911
44	H	4.9521	4.1354	-0.7154
45	H	4.0218	4.0642	0.788
46	H	5.7117	3.4948	0.7619
47	C	-3.666	-3.4737	0.6947
48	H	-4.2992	-3.1214	-0.1324
49	C	-3.0304	-4.8199	0.2718
50	H	-2.4876	-4.7226	-0.6743
51	H	-2.3308	-5.1814	1.0406
52	H	-3.808	-5.586	0.1412
53	C	-4.5395	-3.6612	1.9533
54	H	-4.9519	-2.6998	2.2759
55	H	-5.3666	-4.3578	1.7518
56	H	-3.9465	-4.0757	2.7833
57	O	-2.2394	-2.2344	-1.5023
58	O	2.3766	0.5356	-2.7102
59	H	0.0507	-1.9844	0.7753
60	H	2.4256	-0.0993	0.4793
61	C	2.6534	-2.6694	8.0807
62	C	2.6204	-1.5983	7.1601
63	C	1.6285	-0.6052	7.3087
64	C	0.6968	-0.6791	8.3587
65	C	0.7419	-1.7472	9.2757
66	C	1.7242	-2.7464	9.1318
67	H	3.4111	-3.4431	7.9704
68	H	1.5701	0.2137	6.5985
69	H	-0.0681	0.088	8.4559
70	H	0.0169	-1.8044	10.0848
71	H	1.761	-3.5801	9.8296
72	Cl	5.2559	-0.6773	6.7456
73	C	3.6439	-1.5525	6.0576
74	H	4.0201	-2.5493	5.8238
75	C	3.2985	-0.7992	4.7743
76	H	3.0362	0.2477	4.9717
77	H	4.1488	-0.8033	4.0866
78	O	2.1682	-1.5231	4.1995
79	C	1.8577	-1.232	2.8156
80	O	0.8861	-1.9087	2.36
81	O	2.5929	-0.3413	2.2502

- Lowest energy conformation for **[1·Int1]**.

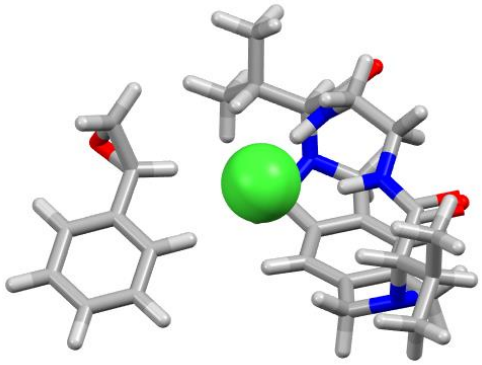


Cartesian coordinates (78 atoms), E (298.15 K) = -1626.141858 Hartree

1	H	-0.6591	1.4977	2.8266
2	C	-0.951	1.5831	1.7844
3	C	-1.6118	1.6186	-1.0054
4	C	-2.1053	0.9631	1.3036
5	C	-0.0998	2.1758	0.8401
6	C	-0.4284	2.2166	-0.5266
7	C	-2.4239	0.9543	-0.0741
8	H	-1.8348	1.5874	-2.0701
9	C	1.3245	2.6447	1.0527
10	H	1.3723	3.5936	1.6149
11	H	1.877	1.8943	1.6301
12	C	0.7361	2.8187	-1.3029
13	H	0.5101	3.8437	-1.6426
14	C	-3.0658	0.0244	2.0218
15	H	-2.6081	-0.5178	2.8543
16	H	-3.9439	0.5646	2.4125
17	C	-3.5906	-0.0198	-0.2776
18	H	-3.5294	-0.6041	-1.1974
19	H	-4.56	0.5032	-0.2583
20	N	-3.5216	-0.9117	0.9377
21	C	-2.648	-2.1483	0.8261
22	H	-2.004	-2.1691	1.717
23	C	-1.7257	-2.1605	-0.4191
24	N	-0.4114	-1.8714	-0.2409
25	C	0.4653	-1.8458	-1.4263
26	H	0.3462	-2.7907	-1.9759
27	H	0.1484	-1.0464	-2.1113
28	C	1.9468	-1.6503	-1.0559
29	H	2.5521	-1.8056	-1.9542
30	H	2.2334	-2.3878	-0.2954
31	N	2.2496	-0.3079	-0.5312
32	C	2.8104	0.6419	-1.3297
33	C	3.0787	2.0719	-0.7617

34	H	3.473	2.5983	-1.6432
35	N	1.8733	2.8219	-0.326
36	H	0.9912	2.2293	-2.1936
37	C	4.2194	2.0754	0.2985
38	H	3.8777	1.5319	1.1917
39	C	5.4687	1.3396	-0.2408
40	H	6.2753	1.3667	0.5052
41	H	5.2519	0.2911	-0.4726
42	H	5.8351	1.8149	-1.1612
43	C	4.5859	3.5199	0.7105
44	H	4.9603	4.0806	-0.1583
45	H	3.7178	4.0586	1.1026
46	H	5.3745	3.5142	1.4767
47	C	-3.5298	-3.4321	0.8402
48	H	-4.1555	-3.3916	-0.0624
49	C	-2.6626	-4.712	0.7748
50	H	-2.0794	-4.7515	-0.1515
51	H	-1.9659	-4.76	1.6256
52	H	-3.2987	-5.6078	0.815
53	C	-4.4424	-3.4609	2.0843
54	H	-5.0264	-2.5368	2.1459
55	H	-5.1317	-4.3167	2.0412
56	H	-3.8473	-3.5585	3.0064
57	O	-2.2107	-2.4504	-1.5663
58	O	3.1392	0.4117	-2.5411
59	H	0.0157	-1.5371	0.6732
60	H	1.9151	-0.1904	0.4531
61	C	-0.7945	-1.3273	5.5599
62	C	0.3605	-1.0981	4.7785
63	C	1.0292	0.1387	4.9076
64	C	0.5619	1.1143	5.8062
65	C	-0.5858	0.8725	6.5875
66	C	-1.2661	-0.3543	6.4588
67	H	-1.316	-2.2784	5.4688
68	H	1.8957	0.3411	4.2876
69	H	1.085	2.0649	5.8905
70	H	-0.9479	1.6307	7.2792
71	H	-2.1574	-0.549	7.0519
72	Cl	1.8133	-3.5215	4.9616
73	C	0.8505	-2.1738	3.8429
74	H	0.0283	-2.7882	3.4696
75	C	1.787	-1.7688	2.6943
76	H	2.6984	-1.3011	3.1186
77	H	2.123	-2.7029	2.1995
78	O	1.0613	-0.8985	1.833

- Lowest energy conformation for **[1·Cl·SO]**.

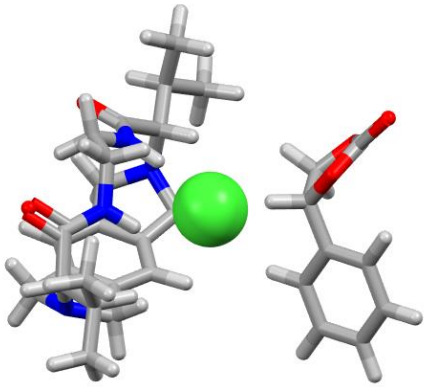


Cartesian coordinates (78 atoms), E (298.15 K) = -1626.155527 Hartree

1	H	-0.6131	1.7511	2.4093
2	C	-0.8919	1.8009	1.3618
3	C	-1.5171	1.7316	-1.4636
4	C	-2.0529	1.182	0.8905
5	C	-0.0203	2.3409	0.406
6	C	-0.3237	2.3157	-0.9686
7	C	-2.3642	1.1373	-0.4863
8	H	-1.7311	1.6638	-2.501
9	C	1.396	2.8423	0.6163
10	H	1.4102	3.8553	1.0524
11	H	1.9474	2.1919	1.3043
12	C	0.8683	2.8649	-1.7472
13	H	0.6751	3.8898	-2.1056
14	C	-3.0372	0.2997	1.6447
15	H	-2.5606	-0.2757	2.4448
16	H	-3.8541	0.8905	2.091
17	C	-3.5907	0.2363	-0.6663
18	H	-3.5496	-0.3929	-1.5584
19	H	-4.5179	0.8301	-0.7014
20	N	-3.6063	-0.6003	0.5866
21	C	-2.9501	-1.956	0.5039
22	H	-2.4449	-2.1211	1.4658
23	C	-1.8864	-2.0617	-0.6221
24	N	-0.5815	-1.8777	-0.2829
25	C	0.4567	-1.9468	-1.3279
26	H	0.4021	-2.9341	-1.8095
27	H	0.2504	-1.2089	-2.1126
28	C	1.8758	-1.7332	-0.7693
29	H	2.5849	-2.092	-1.5224
30	H	2.0035	-2.2997	0.1595
31	N	2.2099	-0.33	-0.4752
32	C	2.7268	0.4872	-1.4403
33	C	3.1228	1.9544	-1.0845
34	H	3.541	2.3182	-2.0335
35	N	1.9949	2.8659	-0.7549

36	H	1.122	2.2523	-2.6211
37	C	4.2764	2.0084	-0.0391
38	H	3.9145	1.6077	0.9191
39	C	5.4617	1.1232	-0.4915
40	H	6.2729	1.1738	0.2473
41	H	5.1667	0.0734	-0.6008
42	H	5.8567	1.4637	-1.4591
43	C	4.7497	3.4619	0.1881
44	H	5.1512	3.8846	-0.7446
45	H	3.9269	4.1046	0.5153
46	H	5.5441	3.4917	0.9469
47	C	-4.0193	-3.075	0.3312
48	H	-4.508	-2.9024	-0.6384
49	C	-3.3662	-4.4774	0.3004
50	H	-2.6882	-4.5827	-0.5532
51	H	-2.7973	-4.6656	1.2236
52	H	-4.1377	-5.2563	0.2201
53	C	-5.0796	-2.9979	1.4498
54	H	-5.5043	-1.9901	1.4993
55	H	-5.8886	-3.7204	1.2681
56	H	-4.6348	-3.233	2.4295
57	O	-2.237	-2.3115	-1.8219
58	O	2.9193	0.0769	-2.6298
59	H	-0.2923	-1.607	0.6685
60	H	1.9924	-0.0272	0.4786
61	Cl	0.9747	-0.8959	2.4922
62	C	0.6851	-0.2263	6.0735
63	C	2.0304	0.1131	6.3469
64	C	2.3894	0.5537	7.64
65	C	1.419	0.6382	8.6551
66	C	0.0808	0.2852	8.3871
67	C	-0.2806	-0.1435	7.0941
68	H	0.4187	-0.5472	5.0673
69	H	3.4184	0.8528	7.8256
70	H	1.7011	0.9852	9.6478
71	H	-0.6705	0.3522	9.172
72	H	-1.314	-0.4081	6.8778
73	O	4.3582	0.7076	5.4613
74	C	4.3076	-0.7895	5.4394
75	H	4.7753	-1.2536	4.5734
76	H	4.4986	-1.2646	6.4011
77	C	3.0412	-0.013	5.253
78	H	2.6469	0.0471	4.2399

- Lowest energy conformation for **[1·Cl⁻·SC]**.

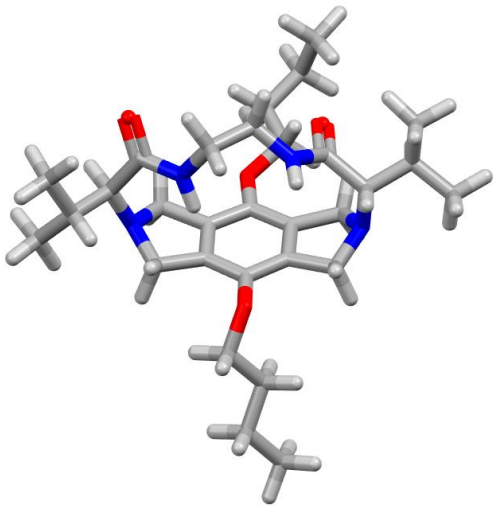


Cartesian coordinates (81 atoms), E (298.15 K) = -1814.735385 Hartree

1	H	-0.1791	1.5038	2.6666
2	C	-0.5325	1.6087	1.6459
3	C	-1.3806	1.683	-1.0925
4	C	-1.7747	1.1016	1.2549
5	C	0.3037	2.1057	0.6368
6	C	-0.1081	2.1493	-0.7088
7	C	-2.1974	1.1303	-0.0926
8	H	-1.6839	1.6695	-2.1373
9	C	1.7677	2.4895	0.741
10	H	1.8948	3.485	1.2022
11	H	2.3197	1.7784	1.3691
12	C	1.0603	2.6237	-1.5683
13	H	0.9235	3.6695	-1.8897
14	C	-2.7701	0.2818	2.0631
15	H	-2.2862	-0.3578	2.8081
16	H	-3.496	0.9247	2.5873
17	C	-3.5096	0.3449	-0.1938
18	H	-3.5987	-0.2522	-1.104
19	H	-4.3796	1.0175	-0.131
20	N	-3.4954	-0.532	1.031
21	C	-2.9581	-1.931	0.8528
22	H	-2.3919	-2.1694	1.7644
23	C	-2.0007	-2.0757	-0.3601
24	N	-0.6609	-2.0165	-0.1223
25	C	0.2842	-2.1255	-1.2493
26	H	0.1077	-3.0827	-1.761
27	H	0.0816	-1.3395	-1.9869
28	C	1.7562	-2.0552	-0.8009
29	H	2.3703	-2.4437	-1.6196
30	H	1.907	-2.6685	0.0941
31	N	2.2361	-0.6978	-0.4914
32	C	2.7446	0.1079	-1.472
33	C	3.283	1.527	-1.1093
34	H	3.6543	1.8888	-2.0783
35	N	2.2568	2.5083	-0.669

36	H	1.1947	2.0158	-2.4716
37	C	4.514	1.4602	-0.1577
38	H	4.1995	1.0449	0.8114
39	C	5.595	0.516	-0.7354
40	H	6.4642	0.4816	-0.0648
41	H	5.221	-0.5069	-0.8574
42	H	5.9348	0.8683	-1.7193
43	C	5.1054	2.868	0.082
44	H	5.4545	3.3029	-0.8658
45	H	4.3612	3.5507	0.5034
46	H	5.9627	2.8124	0.7675
47	C	-4.1226	-2.9587	0.7367
48	H	-4.6752	-2.7133	-0.1814
49	C	-3.5857	-4.4041	0.6057
50	H	-2.9833	-4.5264	-0.3008
51	H	-2.9675	-4.6742	1.4752
52	H	-4.4201	-5.1177	0.5571
53	C	-5.0767	-2.8447	1.944
54	H	-5.4188	-1.8115	2.061
55	H	-5.9501	-3.4988	1.8096
56	H	-4.5715	-3.1489	2.874
57	O	-2.4634	-2.2407	-1.5352
58	O	2.8078	-0.2753	-2.683
59	H	-0.2805	-1.8107	0.8109
60	H	2.1249	-0.4088	0.483
61	C	2.8	-0.3977	5.69
62	C	3.2798	-1.6904	6.0037
63	C	4.068	-1.8799	7.1563
64	C	4.3644	-0.7902	7.9986
65	C	3.879	0.4947	7.6935
66	C	3.0983	0.6859	6.5351
67	H	2.2057	-0.2597	4.7878
68	H	4.4628	-2.866	7.3814
69	H	4.975	-0.9463	8.8858
70	H	4.1089	1.336	8.3444
71	H	2.7263	1.6779	6.2868
72	Cl	1.1786	-1.2646	2.5743
73	C	1.4402	-3.3382	5.1976
74	H	0.7905	-2.6455	5.7295
75	H	1.0186	-3.5908	4.2245
76	O	1.5534	-4.5786	6.0168
77	C	2.8735	-5.0048	6.0427
78	O	3.2697	-6.0533	6.5393
79	O	3.6898	-4.0621	5.4209
80	C	2.9111	-2.8387	5.077
81	H	3.1228	-2.5858	4.0374

- Lowest energy conformation for **3**.



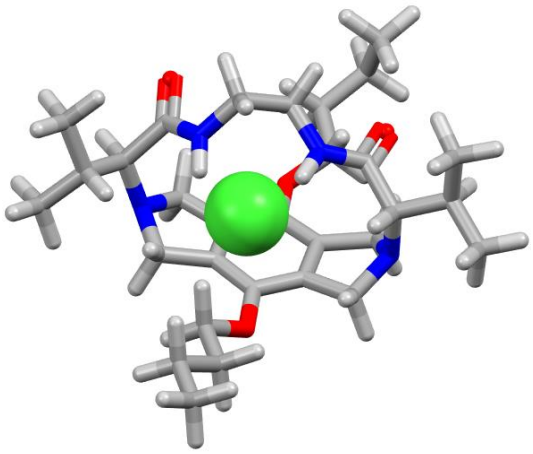
Cartesian coordinates (86 atoms). E (298.15 K) = -1691.051489 Hartree

1	C	-0.5834	1.1158	2.1472
2	C	-1.5569	2.3481	-0.2526
3	C	-1.8331	0.7918	1.612
4	C	0.2111	2.0311	1.4331
5	C	-0.2669	2.6144	0.2503
6	C	-2.3379	1.3949	0.4348
7	C	1.6697	2.4313	1.636
8	H	1.759	3.2184	2.4031
9	H	2.2965	1.596	1.9697
10	C	0.8506	3.3923	-0.4259
11	H	0.7019	4.479	-0.3364
12	C	-2.8011	-0.2886	2.0742
13	H	-2.3015	-1.1888	2.4444
14	H	-3.4508	0.0805	2.8827
15	C	-3.7056	0.7457	0.1467
16	H	-3.9223	0.5903	-0.9072
17	H	-4.5143	1.347	0.5878
18	N	-3.6378	-0.5675	0.8664
19	C	-3.1906	-1.7348	0.037
20	H	-2.7708	-2.4681	0.7422
21	C	-2.0998	-1.3704	-1.0122
22	N	-0.8023	-1.7171	-0.7209
23	C	0.3046	-1.5096	-1.6772
24	H	0.3751	-2.384	-2.343
25	H	0.0535	-0.6485	-2.3012
26	C	1.6763	-1.3065	-0.999
27	H	2.4504	-1.5069	-1.7459
28	H	1.8026	-2.0315	-0.1798
29	N	1.9402	0.0433	-0.4836
30	C	2.7689	0.9217	-1.1573
31	C	3.1335	2.285	-0.4853

32	H	3.3517	2.9355	-1.3429
33	N	2.0799	2.9556	0.303
34	H	0.9158	3.1643	-1.4966
35	C	4.4699	2.1698	0.3282
36	H	4.2751	1.5627	1.2263
37	C	5.5989	1.4756	-0.4675
38	H	6.5223	1.4807	0.127
39	H	5.3587	0.4376	-0.7189
40	H	5.7948	2.0005	-1.411
41	C	4.9288	3.575	0.7834
42	H	5.1943	4.1909	-0.0876
43	H	4.1394	4.097	1.3327
44	H	5.818	3.4981	1.4233
45	C	-4.3973	-2.4148	-0.6766
46	H	-4.825	-1.6744	-1.3681
47	C	-3.9394	-3.637	-1.5077
48	H	-3.2421	-3.352	-2.3033
49	H	-3.4542	-4.3897	-0.8681
50	H	-4.8058	-4.1172	-1.9803
51	C	-5.4764	-2.8267	0.346
52	H	-5.7682	-1.974	0.9661
53	H	-6.3657	-3.2125	-0.1701
54	H	-5.1058	-3.6223	1.0104
55	O	-2.3965	-0.7752	-2.0894
56	O	3.273	0.6191	-2.2741
57	H	-0.6104	-2.2241	0.1361
58	H	1.4308	0.3552	0.3336
59	O	-1.8886	3.0567	-1.4093
60	O	-0.0899	0.4011	3.2654
61	C	-2.9104	2.5522	-2.3487
62	H	-2.7071	1.4982	-2.5629
63	H	-3.905	2.6516	-1.8885
64	C	-2.8204	3.4224	-3.6032
65	H	-2.9524	4.473	-3.3089
66	H	-1.8111	3.3311	-4.0282
67	C	-3.8747	3.0376	-4.67
68	H	-4.8817	3.0915	-4.2264
69	H	-3.8494	3.7927	-5.4688
70	C	-3.6569	1.6394	-5.2927
71	H	-2.6602	1.5693	-5.7497
72	H	-3.7345	0.8385	-4.5471
73	H	-4.4004	1.4405	-6.0759
74	C	0.1225	1.1743	4.507
75	H	0.7165	0.5068	5.1405
76	H	0.7173	2.0731	4.2858
77	C	-1.1955	1.5558	5.1946
78	H	-1.7972	2.1757	4.5143
79	H	-1.7708	0.6401	5.3938

80	C	-0.9588	2.3228	6.5156
81	H	-0.3371	1.7121	7.1887
82	H	-0.387	3.2408	6.309
83	C	-2.2765	2.6909	7.2295
84	H	-2.8535	1.7903	7.4794
85	H	-2.0845	3.2371	8.1622
86	H	-2.9059	3.3256	6.5912

- Lowest energy conformation for **[3·Cl⁻]**.



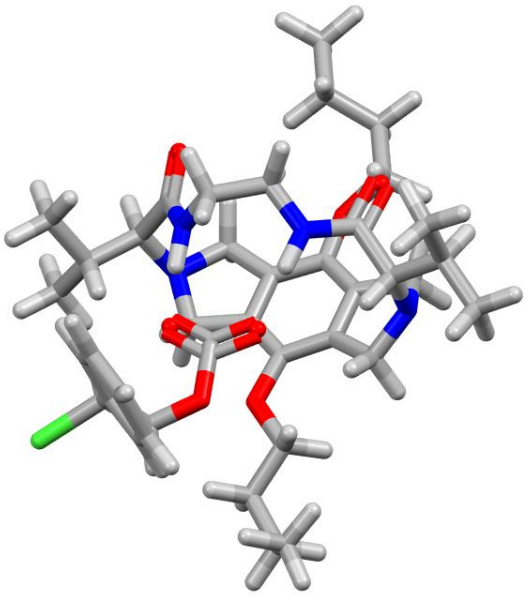
Cartesian coordinates (87 atoms). E (298.15 K) = -1706.129101 Hartree

1	C	-1.5172	2.2199	1.958
2	C	-1.8957	2.723	-0.8425
3	C	-2.6191	1.7226	1.2549
4	C	-0.5183	2.8644	1.2009
5	C	-0.7291	3.1253	-0.1649
6	C	-2.8311	1.9539	-0.1215
7	C	0.9017	3.2854	1.569
8	H	0.9003	4.1954	2.1934
9	H	1.4258	2.5108	2.1331
10	C	0.4998	3.799	-0.7561
11	H	0.3299	4.8782	-0.8984
12	C	-3.6607	0.7414	1.7683
13	H	-3.2445	0.0286	2.4848
14	H	-4.5025	1.2567	2.2571
15	C	-4.0907	1.152	-0.5128
16	H	-4.0802	0.7236	-1.5119
17	H	-4.9899	1.7799	-0.41
18	N	-4.157	0.0678	0.5231
19	C	-3.4367	-1.2207	0.1904
20	H	-2.9147	-1.5395	1.1034
21	C	-2.3779	-1.0802	-0.9344
22	N	-1.0716	-1.0541	-0.5732
23	C	-0.0248	-0.8965	-1.6
24	H	-0.1053	-1.7257	-2.3184
25	H	-0.1932	0.0267	-2.1679
26	C	1.3934	-0.8807	-0.9996
27	H	2.1032	-1.0126	-1.8225
28	H	1.5023	-1.6952	-0.2758
29	N	1.739	0.3697	-0.3038
30	C	2.307	1.4152	-0.9723
31	C	2.7032	2.7143	-0.2004

32	H	3.2105	3.2954	-0.9837
33	N	1.5698	3.5612	0.2635
34	H	0.776	3.3841	-1.7313
35	C	3.7645	2.4385	0.9043
36	H	3.3182	1.8093	1.6891
37	C	4.965	1.6571	0.3189
38	H	5.7185	1.4815	1.099
39	H	4.6599	0.6839	-0.0817
40	H	5.4398	2.2229	-0.495
41	C	4.2519	3.7575	1.5473
42	H	4.7279	4.3971	0.79
43	H	3.4247	4.3253	1.984
44	H	4.9922	3.5515	2.3335
45	C	-4.4607	-2.3324	-0.1906
46	H	-4.9761	-1.991	-1.1
47	C	-3.7484	-3.6692	-0.507
48	H	-3.0777	-3.5729	-1.3681
49	H	-3.1577	-4.0125	0.3553
50	H	-4.487	-4.4498	-0.7387
51	C	-5.5001	-2.5259	0.9332
52	H	-5.9709	-1.5691	1.1805
53	H	-6.2777	-3.2394	0.624
54	H	-5.0235	-2.9224	1.8431
55	O	-2.7374	-0.9979	-2.1602
56	O	2.547	1.3587	-2.2216
57	H	-0.7727	-1.0774	0.418
58	H	1.5018	0.3756	0.6943
59	O	-1.9842	3.1219	-2.1922
60	O	-1.5408	2.0317	3.3487
61	C	-2.6732	2.2507	-3.1572
62	H	-2.4258	1.2043	-2.9521
63	H	-3.7621	2.3853	-3.0571
64	C	-2.2172	2.6687	-4.5566
65	H	-2.4572	3.732	-4.7036
66	H	-1.1238	2.5738	-4.6143
67	C	-2.8778	1.816	-5.6679
68	H	-3.9741	1.872	-5.5677
69	H	-2.6323	2.262	-6.644
70	C	-2.4357	0.3334	-5.6617
71	H	-1.3451	0.2576	-5.7764
72	H	-2.7037	-0.1744	-4.7276
73	H	-2.9009	-0.2165	-6.4923
74	C	-0.2964	1.7649	4.0941
75	H	0.3199	1.0648	3.5176
76	H	0.2325	2.716	4.2692
77	C	-0.7	1.1144	5.417
78	H	-1.3623	1.7897	5.9804
79	H	-1.2717	0.2066	5.1844

80	C	0.5347	0.7409	6.2672
81	H	1.1675	0.0568	5.6837
82	H	1.1365	1.643	6.4659
83	C	0.1518	0.076	7.6062
84	H	-0.422	-0.8441	7.4297
85	H	1.0423	-0.189	8.1934
86	H	-0.4701	0.7467	8.2169
87	Cl	0.4615	-1.0487	2.2875

- Lowest energy conformation for **[3·Int2]**.



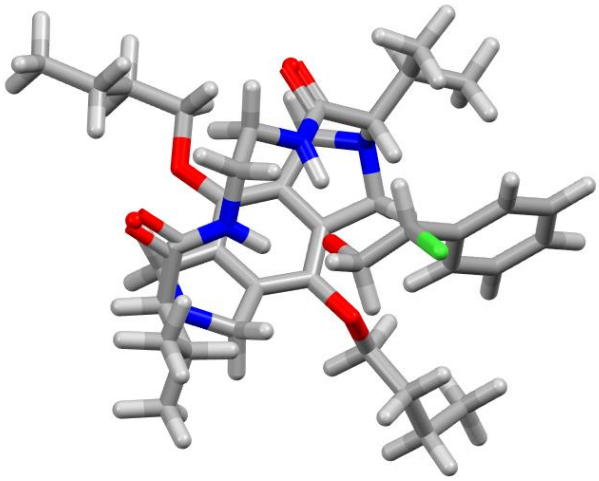
Cartesian coordinates (107 atoms). E (298.15 K) = -2279.366513 Hartree

1	C	-0.6792	2.8836	1.3672
2	C	-1.1517	-2.2925	1.3975
3	C	-1.8745	2.2762	0.9542
4	C	0.3186	3.0686	0.3966
5	C	0.0897	-2.7898	0.9518
6	C	-2.1186	-1.9928	0.4184
7	C	1.7708	3.4415	0.6165
8	H	1.8823	4.5154	0.8383
9	H	2.1929	2.8937	1.4641
10	C	1.371	3.0323	-1.7375
11	H	1.3164	3.977	-2.3013
12	C	-3.0124	1.666	1.7816
13	H	-2.6525	1.1675	2.6833
14	H	-3.7591	2.4229	2.072
15	C	-3.4791	1.2753	-0.501
16	H	-3.5406	0.499	-1.2607
17	H	-4.2879	2.0022	-0.6783
18	N	-3.6571	0.6837	0.8622
19	C	-3.1909	-0.7395	1.0396
20	H	-2.7815	-0.8111	2.0557
21	C	-2.0731	-1.147	0.0435
22	N	-0.7927	-1.0952	0.4858
23	C	0.3055	-1.4613	-0.4261
24	H	0.1465	-2.4956	-0.7654
25	H	0.2788	-0.8362	-1.3258
26	C	1.6964	-1.353	0.2287
27	H	2.3803	-1.9745	-0.3622
28	H	1.6637	-1.7382	1.2546

29	N	2.2496	0.0086	0.2853
30	C	2.8172	0.5686	-0.8202
31	C	3.4329	1.9988	-0.728
32	H	3.9468	2.0966	-1.695
33	N	2.4387	3.1088	-0.6831
34	H	1.5803	2.2331	-2.4562
35	C	4.5244	2.1088	0.3761
36	H	4.0634	1.9415	1.3602
37	C	5.6018	1.0163	0.1762
38	H	6.3641	1.0872	0.9641
39	H	5.1697	0.0096	0.212
40	H	6.1025	1.135	-0.7955
41	C	5.1795	3.5087	0.3734
42	H	5.6631	3.7042	-0.595
43	H	4.4399	4.2981	0.5375
44	H	5.9466	3.5746	1.1582
45	C	-4.3884	-1.7287	0.933
46	H	-4.7867	-1.6444	-0.0885
47	C	-3.9274	-3.1897	1.1515
48	H	-3.2132	-3.501	0.3818
49	H	-3.4514	-3.3063	2.1367
50	H	-4.7881	-3.8726	1.113
51	C	-5.4977	-1.3559	1.9391
52	H	-5.785	-0.3068	1.8151
53	H	-6.3839	-1.9906	1.7934
54	H	-5.1503	-1.4975	2.9743
55	O	-2.3652	-1.5083	-1.1483
56	O	2.8612	-0.0462	-1.9363
57	H	-0.5716	-0.726	1.4295
58	H	2.2085	0.4639	1.2115
59	C	3.4439	-1.8821	6.4649
60	C	2.6966	-0.6974	6.65
61	C	1.6978	-0.674	7.6483
62	C	1.4616	-1.8047	8.4488
63	C	2.2182	-2.9783	8.2623
64	C	3.2102	-3.0151	7.2633
65	H	4.2077	-1.9121	5.6903
66	H	1.0926	0.2164	7.7875
67	H	0.6835	-1.7757	9.2085
68	H	2.0305	-3.8543	8.8799
69	H	3.7919	-3.9205	7.1044
70	Cl	4.3857	1.565	6.6492
71	C	2.9928	0.4921	5.778
72	H	3.4781	0.2079	4.8457
73	C	1.8609	1.4881	5.4963
74	H	1.4959	1.9432	6.422
75	H	2.2349	2.2646	4.8233
76	O	-0.3207	3.2875	2.6653

77	O	-1.2742	2.1449	-2.7933
78	C	-1.3156	3.3519	3.7394
79	H	-1.4593	2.3473	4.1502
80	H	-2.2677	3.7349	3.3422
81	C	-0.761	4.3116	4.7958
82	H	-0.5214	5.2637	4.3016
83	H	0.1823	3.904	5.1816
84	C	-2.0938	1.0652	-3.3719
85	H	-1.9575	0.139	-2.7995
86	H	-3.1534	1.3608	-3.3315
87	C	-1.6435	0.8896	-4.8247
88	H	-2.37	0.2298	-5.3275
89	H	-1.6887	1.8664	-5.3303
90	C	-0.2257	0.2941	-4.9589
91	H	0.4844	0.933	-4.4203
92	H	-0.198	-0.6861	-4.4608
93	C	0.2185	0.1425	-6.4285
94	H	0.2258	1.1165	-6.9392
95	H	1.2304	-0.2793	-6.4927
96	H	-0.4612	-0.5213	-6.9835
97	C	-1.7396	4.5658	5.9676
98	H	-1.3123	5.3494	6.6116
99	H	-2.6859	4.9709	5.5738
100	C	-2.0348	3.3162	6.8286
101	H	-2.5465	2.5364	6.2522
102	H	-1.1024	2.8789	7.2106
103	H	-2.6698	3.571	7.6886
104	O	0.7006	0.8215	4.9102
105	C	0.8082	0.4477	3.5172
106	O	-0.2542	-0.0675	3.0482
107	O	1.9414	0.6732	2.9553

- Lowest energy conformation for **[3·Int1]**.



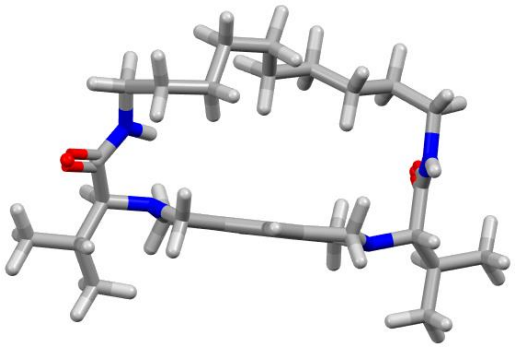
Cartesian coordinates (104 atoms). E (298.15 K) = -2090.782308 Hartree

1	C	-0.6294	2.3459	1.7421
2	C	-1.287	2.2232	-1.0356
3	C	-1.8289	1.786	1.3056
4	C	0.299	2.7351	0.7668
5	C	-0.0343	2.6987	-0.5906
6	C	-2.1707	1.7025	-0.0691
7	C	1.7758	3.0115	0.9437
8	H	1.9651	3.9655	1.4647
9	H	2.214	2.2147	1.5558
10	C	1.1761	3.0752	-1.4251
11	H	1.0629	4.0734	-1.8788
12	C	-2.8374	0.9744	2.1115
13	H	-2.3864	0.4532	2.9583
14	H	-3.6605	1.6025	2.4921
15	C	-3.4566	0.848	-0.1442
16	H	-3.5421	0.2074	-1.0169
17	H	-4.3521	1.4868	-0.0823
18	N	-3.3966	0.019	1.1036
19	C	-2.6101	-1.2788	1.0112
20	H	-1.9303	-1.3088	1.873
21	C	-1.7522	-1.4139	-0.2729
22	N	-0.4055	-1.3298	-0.1528
23	C	0.4225	-1.452	-1.3684
24	H	0.1902	-2.4061	-1.8646
25	H	0.1608	-0.6582	-2.0822
26	C	1.9311	-1.3868	-1.0632
27	H	2.4827	-1.6068	-1.9823
28	H	2.185	-2.14	-0.3055
29	N	2.3667	-0.067	-0.5779
30	C	3.086	0.7705	-1.3747
31	C	3.4607	2.1945	-0.8516
32	H	3.9002	2.6575	-1.7478

33	N	2.3116	3.042	-0.4504
34	H	1.3341	2.3679	-2.2493
35	C	4.5915	2.1525	0.2185
36	H	4.1933	1.7033	1.1399
37	C	5.7705	1.2713	-0.2556
38	H	6.5742	1.2821	0.4938
39	H	5.4627	0.2316	-0.4115
40	H	6.1791	1.6419	-1.2058
41	C	5.0895	3.5804	0.5428
42	H	5.5319	4.0418	-0.3523
43	H	4.2714	4.2253	0.8784
44	H	5.8603	3.5519	1.3263
45	C	-3.5812	-2.4938	1.1178
46	H	-4.2537	-2.4349	0.2498
47	C	-2.8134	-3.8357	1.0517
48	H	-2.2846	-3.9496	0.0986
49	H	-2.0791	-3.906	1.8677
50	H	-3.5103	-4.6795	1.1557
51	C	-4.4193	-2.4161	2.4114
52	H	-4.9398	-1.4544	2.4677
53	H	-5.1637	-3.2254	2.4386
54	H	-3.7788	-2.5179	3.3005
55	O	-2.3217	-1.6224	-1.4035
56	O	3.4686	0.4462	-2.5481
57	H	0.1032	-1.0471	0.7389
58	H	2.0192	0.1205	0.3981
59	C	-0.3121	-3.1785	4.9237
60	C	0.3067	-2.088	4.2678
61	C	-0.1641	-0.7801	4.525
62	C	-1.2148	-0.5778	5.442
63	C	-1.8152	-1.6654	6.1027
64	C	-1.3619	-2.973	5.8345
65	H	0.0513	-4.1859	4.7347
66	H	0.2464	0.0597	3.9725
67	H	-1.5716	0.4337	5.6263
68	H	-2.6288	-1.5004	6.8069
69	H	-1.8223	-3.824	6.3329
70	Cl	2.8473	-3.3648	4.2297
71	C	1.4348	-2.3285	3.289
72	H	1.1581	-3.046	2.512
73	C	2.1147	-1.0947	2.6701
74	H	2.4576	-0.4371	3.4936
75	H	3.0258	-1.4468	2.1456
76	O	1.1998	-0.4383	1.7969
77	O	-0.2823	2.3995	3.119
78	O	-1.4731	2.2821	-2.4269
79	C	-0.9189	3.4975	3.861
80	H	-2.0051	3.3247	3.9076

81	H	-0.7443	4.4483	3.3309
82	C	-0.2893	3.5329	5.2561
83	H	0.7978	3.6297	5.1313
84	H	-0.463	2.5678	5.7522
85	C	-2.4871	1.4474	-3.0897
86	H	-2.3384	0.3952	-2.8141
87	H	-3.488	1.7695	-2.7647
88	C	-2.3188	1.653	-4.5966
89	H	-3.1586	1.1482	-5.1019
90	H	-2.4023	2.727	-4.8223
91	C	-0.9832	1.1068	-5.1452
92	H	-0.1546	1.6014	-4.6236
93	H	-0.9082	0.0352	-4.9064
94	C	-0.8398	1.3097	-6.6676
95	H	-0.8858	2.3771	-6.9282
96	H	0.1192	0.9167	-7.0306
97	H	-1.6446	0.7964	-7.2144
98	C	-0.8191	4.6838	6.1441
99	H	-0.2192	4.7141	7.0658
100	H	-0.6532	5.6463	5.6345
101	C	-2.3122	4.5557	6.5247
102	H	-2.9641	4.6229	5.6443
103	H	-2.5074	3.5901	7.0118
104	H	-2.6113	5.3511	7.2211

- Lowest energy conformation for **2·**.

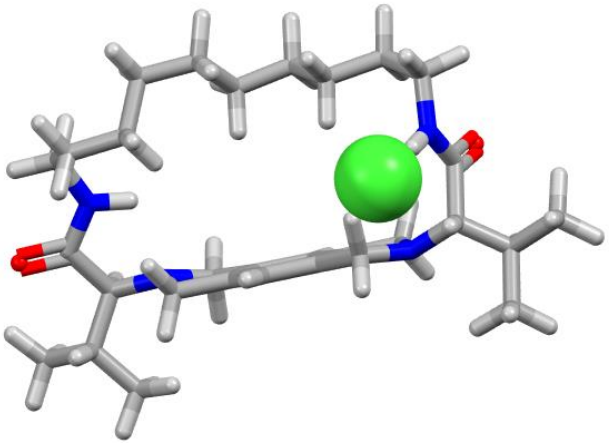


Cartesian coordinates (84 atoms). E (298.15 K) = -1540.660439 Hartree

1	H	2.002	-3.1779	1.4651
2	C	1.8259	-2.158	1.1297
3	C	1.3547	0.5206	0.2445
4	C	1.422	-1.1579	2.029
5	C	1.9829	-1.8045	-0.2219
6	C	1.7403	-0.4849	-0.6565
7	C	1.1995	0.1668	1.5928
8	H	1.1733	1.5389	-0.0933
9	C	2.3683	-2.6843	-1.3971
10	H	3.3223	-3.2064	-1.2288
11	H	1.6081	-3.4596	-1.5937
12	C	1.9054	-0.3941	-2.159
13	H	2.5685	0.4292	-2.4674
14	C	1.1632	-1.2583	3.5234
15	H	0.5095	-2.1038	3.7856
16	H	2.1089	-1.3948	4.0769
17	C	0.8017	1.0397	2.7674
18	H	-0.0752	1.6698	2.5585
19	H	1.6258	1.7211	3.0492
20	N	0.4892	0.0338	3.8113
21	C	0.2049	0.4677	5.1886
22	H	0.0692	-0.4548	5.7776
23	C	-1.1856	1.1921	5.1966
24	N	-2.075	0.6799	4.2876
25	C	-3.4336	1.2066	4.1033
26	H	-4.1268	0.3617	3.9978
27	C	-1.3814	-2.5075	-4.787
28	H	-1.9335	-1.701	-5.2878
29	N	0.0003	-2.0248	-4.5772
30	C	1.0198	-2.8476	-4.1525
31	C	2.3947	-2.1656	-3.9125
32	H	2.4607	-1.2636	-4.542
33	N	2.489	-1.7082	-2.5145
34	H	0.9189	-0.2138	-2.6343
35	C	3.5612	-3.1082	-4.3163
36	H	3.4664	-4.0241	-3.7161
37	C	3.4553	-3.5089	-5.8057

38	H	3.5021	-2.623	-6.4571
39	H	4.2904	-4.1655	-6.0822
40	H	2.5249	-4.0487	-6.0143
41	C	4.9259	-2.4497	-4.023
42	H	4.9901	-2.1177	-2.9815
43	H	5.7433	-3.1563	-4.2196
44	H	5.0831	-1.5708	-4.666
45	C	1.2962	1.3226	5.9194
46	H	1.2156	2.358	5.557
47	C	1.0429	1.3381	7.4472
48	H	1.8104	1.9383	7.9548
49	H	0.0628	1.7623	7.6756
50	H	1.0947	0.3179	7.8581
51	C	2.7293	0.8104	5.6437
52	H	3.4553	1.4527	6.1598
53	H	2.8659	-0.2111	6.0276
54	H	2.9861	0.8092	4.5783
55	O	-1.4737	2.1401	5.9771
56	O	0.8241	-4.0698	-3.8966
57	H	-1.6873	-0.0124	3.6514
58	H	0.2143	-1.0585	-4.7892
59	H	-3.6941	1.7467	5.0193
60	H	-1.3459	-3.3681	-5.4684
61	C	-2.109	-2.937	-3.4931
62	H	-1.5515	-3.7723	-3.0533
63	C	-3.5564	2.162	2.8892
64	H	-2.8528	2.9922	3.0417
65	H	-3.0943	-3.3324	-3.7868
66	H	-4.568	2.5977	2.8955
67	C	-2.2983	-1.8264	-2.4387
68	H	-1.3233	-1.3733	-2.2012
69	H	-2.9324	-1.0241	-2.8475
70	C	-3.2955	1.4932	1.5172
71	H	-2.347	0.9379	1.5584
72	H	-3.1539	2.2768	0.7568
73	C	-2.9174	-2.3875	-1.1369
74	H	-2.29	-3.2262	-0.7973
75	H	-3.9093	-2.8138	-1.3607
76	C	-4.437	0.5582	1.0499
77	H	-4.7006	-0.1444	1.8561
78	H	-5.3345	1.1701	0.8686
79	C	-3.0521	-1.3695	0.0188
80	H	-3.3346	-1.9176	0.9326
81	H	-2.0666	-0.9216	0.2164
82	C	-4.1065	-0.2622	-0.2212
83	H	-3.7691	0.4184	-1.0183
84	H	-5.0309	-0.7367	-0.5874

- Lowest energy conformation for **[2·Cl⁻]·**.



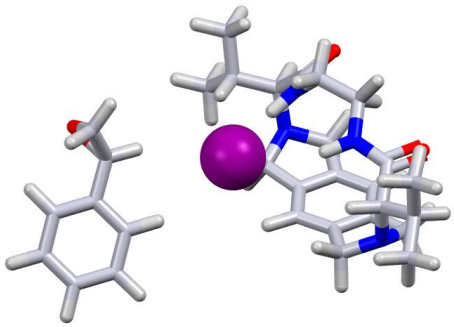
Cartesian coordinates (85 atoms). E (298.15 K) = -1555.727275 Hartree

1	H	1.8598	-3.1968	1.4499
2	C	1.7427	-2.1639	1.1261
3	C	1.4159	0.542	0.2665
4	C	1.361	-1.1585	2.0309
5	C	1.9559	-1.8008	-0.2149
6	C	1.7864	-0.464	-0.6417
7	C	1.2075	0.1781	1.6065
8	H	1.2823	1.5685	-0.0685
9	C	2.3294	-2.6819	-1.3932
10	H	3.2469	-3.2628	-1.1976
11	H	1.5357	-3.4154	-1.6179
12	C	2.0264	-0.3507	-2.1288
13	H	2.7727	0.4206	-2.374
14	C	1.0587	-1.2697	3.5161
15	H	0.3515	-2.0817	3.7473
16	H	1.9788	-1.4663	4.0962
17	C	0.8138	1.055	2.781
18	H	-0.0386	1.714	2.5579
19	H	1.651	1.7101	3.0868
20	N	0.4496	0.053	3.8153
21	C	0.1711	0.4735	5.1951
22	H	0.0232	-0.4536	5.7746
23	C	-1.2114	1.215	5.2224
24	N	-2.0739	0.785	4.2509
25	C	-3.4133	1.3465	4.0401
26	H	-4.138	0.5238	3.9685
27	C	-1.3601	-2.5975	-4.7348
28	H	-1.9219	-1.7992	-5.2368
29	N	-0.0036	-2.0824	-4.5188
30	C	1.0255	-2.8698	-4.114
31	C	2.3793	-2.1359	-3.9027
32	H	2.3618	-1.215	-4.5021
33	N	2.5307	-1.7059	-2.4948

34	H	1.1183	-0.0633	-2.6863
35	C	3.5679	-3.0182	-4.3759
36	H	3.5513	-3.9451	-3.7833
37	C	3.4069	-3.4075	-5.8638
38	H	3.3391	-2.5101	-6.4963
39	H	4.271	-3.9964	-6.2047
40	H	2.5038	-4.0083	-6.018
41	C	4.9115	-2.2943	-4.1434
42	H	4.992	-1.96	-3.103
43	H	5.7586	-2.957	-4.3752
44	H	4.9902	-1.4064	-4.7884
45	C	1.2818	1.2982	5.9345
46	H	1.2304	2.3365	5.5744
47	C	1.0336	1.3144	7.4633
48	H	1.821	1.8891	7.9715
49	H	0.0648	1.7625	7.6938
50	H	1.0572	0.2903	7.8678
51	C	2.6996	0.7469	5.654
52	H	3.4465	1.3696	6.1655
53	H	2.8072	-0.2781	6.0381
54	H	2.948	0.7343	4.5876
55	O	-1.5137	2.1018	6.071
56	O	0.899	-4.1184	-3.8658
57	H	-1.6642	0.132	3.5846
58	H	0.1608	-1.0659	-4.7207
59	H	-3.6547	1.9348	4.9315
60	H	-1.3151	-3.4666	-5.4081
61	C	-2.0876	-3.0336	-3.4403
62	H	-1.5084	-3.8497	-2.9894
63	C	-3.4975	2.244	2.7797
64	H	-2.7702	3.0601	2.8972
65	H	-3.0687	-3.4515	-3.725
66	H	-4.4967	2.7083	2.7555
67	C	-2.2907	-1.9069	-2.4062
68	H	-1.322	-1.433	-2.1936
69	H	-2.9322	-1.1212	-2.8335
70	C	-3.2462	1.5039	1.4429
71	H	-2.3072	0.9362	1.5077
72	H	-3.0891	2.246	0.6458
73	C	-2.8974	-2.4465	-1.0903
74	H	-2.2606	-3.2727	-0.7361
75	H	-3.8891	-2.8858	-1.2962
76	C	-4.4006	0.5655	1.0167
77	H	-4.6671	-0.1059	1.8491
78	H	-5.2925	1.1816	0.8172
79	C	-3.0306	-1.4047	0.0446
80	H	-3.3143	-1.9276	0.9745
81	H	-2.0437	-0.9538	0.2253

82	C	-4.0804	-0.3005	-0.2264
83	H	-3.7404	0.3481	-1.047
84	H	-5.0093	-0.7819	-0.5734
85	Cl	0.3974	0.9527	-5.0551

- Lowest energy conformation for **[1·SO·I⁻]·**.

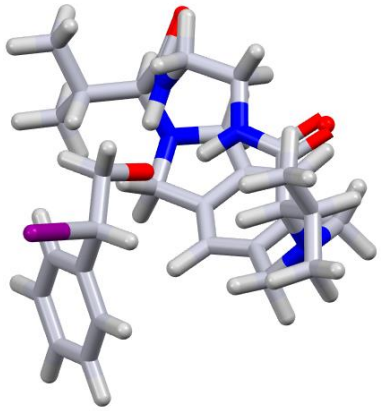


Cartesian coordinates (78 atoms). E (298.15 K) = -1622.601684Hartree

1	H	-0.8674	1.562	2.2136
2	C	-1.1166	1.652	1.1608
3	C	-1.6702	1.719	-1.6531
4	C	-2.2498	1.031	0.626
5	C	-0.2337	2.2624	0.2575
6	C	-0.5041	2.3057	-1.124
7	C	-2.5258	1.0542	-0.7591
8	H	-1.8587	1.709	-2.7247
9	C	1.1566	2.8069	0.5301
10	H	1.116	3.7992	1.0095
11	H	1.7174	2.1504	1.2045
12	C	0.6849	2.9427	-1.839
13	H	0.4622	3.9819	-2.1328
14	C	-3.2487	0.1061	1.3076
15	H	-2.8007	-0.5001	2.1016
16	H	-4.0865	0.6712	1.7479
17	C	-3.7367	0.1505	-1.0167
18	H	-3.6675	-0.4306	-1.9391
19	H	-4.6695	0.7357	-1.0425
20	N	-3.774	-0.75	0.1913
21	C	-3.0855	-2.0847	0.0548
22	H	-2.6313	-2.3054	1.0313
23	C	-1.9628	-2.0971	-1.0176
24	N	-0.6732	-1.9274	-0.6041
25	C	0.4139	-1.917	-1.6026
26	H	0.4088	-2.8822	-2.1294
27	H	0.2159	-1.1509	-2.3601
28	C	1.8045	-1.6914	-0.9812
29	H	2.5457	-2.0232	-1.717
30	H	1.917	-2.2828	-0.0652
31	N	2.1081	-0.2931	-0.6388
32	C	2.5539	0.5849	-1.5871
33	C	2.9385	2.0366	-1.168
34	H	3.3653	2.4444	-2.0948
35	N	1.7903	2.9198	-0.8223
36	H	0.9787	2.3972	-2.7438
37	C	4.0723	2.0618	-0.101
38	H	3.7041	1.6091	0.8315

39	C	5.2806	1.2207	-0.5764
40	H	6.0766	1.2429	0.1797
41	H	5.0057	0.1732	-0.7454
42	H	5.6893	1.6189	-1.5162
43	C	4.5138	3.5106	0.2052
44	H	4.9119	3.9912	-0.7003
45	H	3.676	4.1179	0.5606
46	H	5.3029	3.5158	0.97
47	C	-4.1195	-3.2093	-0.2515
48	H	-4.5616	-2.9777	-1.2312
49	C	-3.4359	-4.5943	-0.346
50	H	-2.7019	-4.6238	-1.1585
51	H	-2.9253	-4.8458	0.596
52	H	-4.1843	-5.3762	-0.5378
53	C	-5.2372	-3.2309	0.8124
54	H	-5.6901	-2.2391	0.9084
55	H	-6.0168	-3.9567	0.5392
56	H	-4.8371	-3.5235	1.7956
57	O	-2.2439	-2.2617	-2.2474
58	O	2.6741	0.2416	-2.8056
59	H	-0.4434	-1.7377	0.3735
60	H	1.9906	-0.0353	0.3432
61	C	1.2679	0.3786	6.9158
62	C	2.6188	0.1548	7.2663
63	C	3.0871	0.5739	8.5314
64	C	2.2117	1.1923	9.4428
65	C	0.8599	1.3998	9.0986
66	C	0.394	0.9936	7.8323
67	H	0.9138	0.0729	5.9325
68	H	4.1391	0.4383	8.7728
69	H	2.582	1.5195	10.4129
70	H	0.1825	1.8798	9.8031
71	H	-0.6446	1.1592	7.5546
72	O	5.0077	-0.4033	6.5466
73	C	4.3257	-1.734	6.6568
74	H	4.5875	-2.4512	5.8816
75	H	4.2532	-2.125	7.671
76	C	3.5219	-0.5246	6.2873
77	H	3.2461	-0.4242	5.2387
78	I	1.1838	-0.9904	2.8477

- Lowest energy conformation for **[1·Int1(I)]·**.

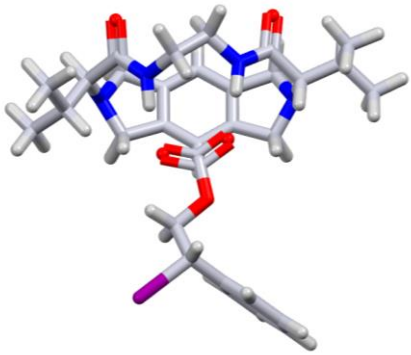


Cartesian coordinates (78 atoms). E (298.15 K) = -1622.585156 Hartree

1	H	-0.8434	1.22	2.92
2	C	-1.1115	1.3625	1.8777
3	C	-1.7044	1.5679	-0.9205
4	C	-2.2406	0.7533	1.3273
5	C	-0.249	2.0296	0.9957
6	C	-0.544	2.1522	-0.3739
7	C	-2.5268	0.831	-0.0552
8	H	-1.9018	1.6039	-1.9901
9	C	1.1581	2.515	1.2761
10	H	1.1668	3.4307	1.8922
11	H	1.7122	1.7475	1.8281
12	C	0.6273	2.8266	-1.0779
13	H	0.3892	3.8685	-1.3513
14	C	-3.2021	-0.2457	1.9576
15	H	-2.7531	-0.8398	2.7592
16	H	-4.0953	0.2543	2.3674
17	C	-3.6752	-0.1408	-0.3514
18	H	-3.5847	-0.662	-1.3061
19	H	-4.6514	0.3689	-0.3216
20	N	-3.6231	-1.1108	0.8035
21	C	-2.7397	-2.3325	0.6275
22	H	-2.1248	-2.4192	1.5352
23	C	-1.7776	-2.2458	-0.5847
24	N	-0.4731	-1.9548	-0.3448
25	C	0.4402	-1.833	-1.4962
26	H	0.3569	-2.7401	-2.1119
27	H	0.1292	-0.9947	-2.1356
28	C	1.9061	-1.638	-1.0669
29	H	2.5411	-1.7305	-1.9531
30	H	2.1805	-2.4145	-0.3419
31	N	2.1725	-0.3246	-0.4559
32	C	2.7348	0.6812	-1.183
33	C	2.9666	2.0779	-0.5236
34	H	3.3739	2.6624	-1.3615

35	N	1.7397	2.7827	-0.0741
36	H	0.915	2.3058	-2.0007
37	C	4.0809	2.0336	0.5637
38	H	3.7269	1.4289	1.4119
39	C	5.3565	1.3556	0.0102
40	H	6.1425	1.3437	0.7783
41	H	5.1643	0.3222	-0.2996
42	H	5.7388	1.8997	-0.8648
43	C	4.4099	3.4548	1.0766
44	H	4.7969	4.0764	0.256
45	H	3.522	3.9526	1.4783
46	H	5.1781	3.4132	1.8622
47	C	-3.6134	-3.6168	0.5121
48	H	-4.2015	-3.5121	-0.4105
49	C	-2.7363	-4.8855	0.388
50	H	-2.1095	-4.8509	-0.5096
51	H	-2.0814	-4.9995	1.2651
52	H	-3.3684	-5.7827	0.3262
53	C	-4.5762	-3.7411	1.7116
54	H	-5.1694	-2.8267	1.8157
55	H	-5.2562	-4.5949	1.5768
56	H	-4.0195	-3.9037	2.6481
57	O	-2.2208	-2.458	-1.7649
58	O	3.0933	0.5283	-2.3976
59	H	-0.0825	-1.6835	0.6014
60	H	1.8149	-0.2651	0.522
61	C	-0.5076	-0.5255	5.5588
62	C	0.6599	-0.7423	4.7915
63	C	1.6635	0.2544	4.7979
64	C	1.5049	1.4278	5.554
65	C	0.3382	1.6307	6.319
66	C	-0.6704	0.6475	6.3167
67	H	-1.2859	-1.2867	5.5653
68	H	2.56	0.1104	4.2035
69	H	2.2845	2.1868	5.543
70	H	0.2159	2.5413	6.902
71	H	-1.5778	0.7949	6.8985
72	C	0.8049	-2.0104	3.999
73	H	-0.1581	-2.4961	3.8255
74	C	1.6358	-1.9787	2.706
75	H	2.6674	-1.6428	2.9297
76	H	1.7204	-3.016	2.3261
77	O	0.9351	-1.1062	1.8306
78	I	1.7572	-3.6523	5.4361

- Lowest energy conformation for **[1·Int2(I)]·**.

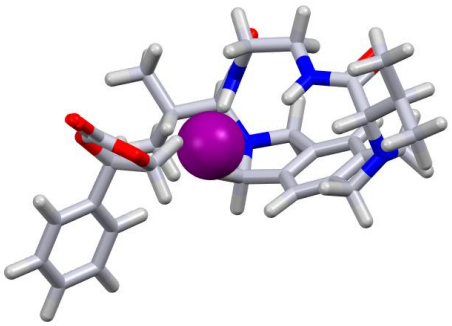


Cartesian coordinates (81 atoms). E (298.15 K) = -1811.16259 Hartree

1	H	0.0679	1.1347	3.0308
2	C	-0.4126	1.3179	2.0733
3	C	-1.6041	1.6814	-0.5058
4	C	-1.6166	0.6915	1.7356
5	C	0.2158	2.0876	1.0843
6	C	-0.365	2.2684	-0.1862
7	C	-2.2105	0.8693	0.467
8	H	-2.0357	1.7836	-1.4994
9	C	1.6072	2.694	1.1054
10	H	1.6252	3.6389	1.675
11	H	2.3279	2.0153	1.5696
12	C	0.6127	3.0429	-1.0677
13	H	0.3017	4.095	-1.1797
14	C	-2.3925	-0.3735	2.4987
15	H	-1.7375	-1.061	3.043
16	H	-3.0929	0.077	3.2217
17	C	-3.4303	-0.0534	0.3779
18	H	-3.5594	-0.5181	-0.6026
19	H	-4.3547	0.49	0.6314
20	N	-3.1737	-1.0913	1.4373
21	C	-2.5558	-2.3849	0.9707
22	H	-1.8978	-2.7265	1.781
23	C	-1.6958	-2.2204	-0.3126
24	N	-0.3591	-2.0396	-0.15
25	C	0.4939	-1.8316	-1.3329
26	H	0.412	-2.7134	-1.986
27	H	0.1266	-0.9827	-1.9204
28	C	1.9773	-1.6119	-0.9733
29	H	2.5643	-1.8456	-1.8697
30	H	2.2735	-2.2936	-0.1675
31	N	2.3265	-0.2456	-0.5498
32	C	2.5187	0.7342	-1.4779
33	C	2.969	2.1534	-1.0118
34	H	3.1727	2.6621	-1.9646
35	N	1.9209	2.9684	-0.3332
36	H	0.7083	2.6146	-2.0725

37	C	4.3121	2.1135	-0.2245
38	H	4.1688	1.5428	0.7041
39	C	5.3979	1.3858	-1.0528
40	H	6.3441	1.3572	-0.4952
41	H	5.1088	0.3538	-1.2821
42	H	5.5773	1.9055	-2.0049
43	C	4.786	3.5386	0.14
44	H	4.9563	4.1318	-0.7705
45	H	4.0405	4.0668	0.742
46	H	5.7301	3.4973	0.702
47	C	-3.6475	-3.4714	0.7495
48	H	-4.2896	-3.1205	-0.0712
49	C	-3.0176	-4.819	0.3229
50	H	-2.4877	-4.725	-0.6308
51	H	-2.3075	-5.1777	1.0835
52	H	-3.7969	-5.5856	0.2059
53	C	-4.507	-3.6551	2.0182
54	H	-4.9137	-2.6922	2.3438
55	H	-5.3377	-4.3503	1.8273
56	H	-3.9055	-4.0694	2.8423
57	O	-2.2413	-2.2397	-1.4658
58	O	2.3606	0.5233	-2.7248
59	H	0.0718	-1.9861	0.7882
60	H	2.4444	-0.0984	0.4663
61	C	2.564	-2.7232	7.9885
62	C	2.5804	-1.5859	7.149
63	C	1.5925	-0.5929	7.3355
64	C	0.6199	-0.7321	8.3397
65	C	0.6162	-1.8667	9.1749
66	C	1.5924	-2.8656	8.9932
67	H	3.3153	-3.4987	7.8497
68	H	1.5727	0.2802	6.6903
69	H	-0.1392	0.0367	8.4649
70	H	-0.1407	-1.9742	9.9489
71	H	1.5919	-3.7508	9.6256
72	C	3.6326	-1.4769	6.082
73	H	4.0508	-2.4549	5.8377
74	C	3.2829	-0.717	4.7997
75	H	2.9832	0.3193	5
76	H	4.1348	-0.6894	4.1144
77	O	2.1778	-1.47	4.2092
78	C	1.8903	-1.2081	2.8135
79	O	0.9311	-1.9009	2.3564
80	O	2.6281	-0.3234	2.2421
81	I	5.494	-0.4375	6.9484

- Lowest energy conformation for **[1·SC·I]·**.

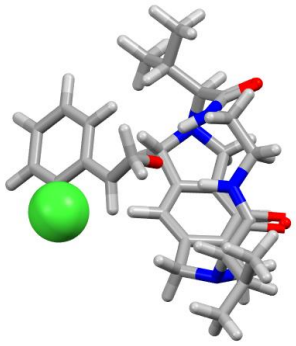


Cartesian coordinates (81 atoms). E (298.15 K) = -1811.172423 Hartree

1	H	-0.2605	1.5514	2.3963
2	C	-0.6234	1.6548	1.378
3	C	-1.5087	1.756	-1.3487
4	C	-1.8667	1.1401	0.996
5	C	0.1942	2.1739	0.3638
6	C	-0.2355	2.2279	-0.9765
7	C	-2.309	1.1865	-0.3446
8	H	-1.8281	1.7571	-2.3888
9	C	1.6474	2.6046	0.4551
10	H	1.7413	3.6111	0.8963
11	H	2.2354	1.9278	1.0844
12	C	0.9134	2.7381	-1.8429
13	H	0.7565	3.7891	-2.136
14	C	-2.8575	0.3197	1.8102
15	H	-2.3709	-0.3337	2.5415
16	H	-3.566	0.9659	2.3536
17	C	-3.6298	0.4152	-0.4364
18	H	-3.7349	-0.1726	-1.351
19	H	-4.4912	1.0971	-0.3579
20	N	-3.6099	-0.4723	0.7802
21	C	-3.0999	-1.8766	0.5776
22	H	-2.5637	-2.1502	1.4974
23	C	-2.1164	-2.0055	-0.6164
24	N	-0.7786	-1.9827	-0.3486
25	C	0.1912	-2.0706	-1.4573
26	H	0.0457	-3.0309	-1.9729
27	H	-0.0192	-1.2891	-2.1956
28	C	1.6555	-1.9715	-0.9899
29	H	2.281	-2.3814	-1.7902
30	H	1.8078	-2.5589	-0.0774
31	N	2.1277	-0.603	-0.7166
32	C	2.5659	0.2048	-1.7318
33	C	3.1312	1.6224	-1.4081
34	H	3.4806	1.9636	-2.3923
35	N	2.1251	2.6242	-0.9625
36	H	1.0457	2.1534	-2.7611

37	C	4.3844	1.5615	-0.4855
38	H	4.0944	1.1608	0.4975
39	C	5.4457	0.6044	-1.0785
40	H	6.329	0.5692	-0.427
41	H	5.0628	-0.4173	-1.1823
42	H	5.7667	0.9464	-2.0725
43	C	4.9881	2.9692	-0.2785
44	H	5.3123	3.3921	-1.2404
45	H	4.2587	3.6598	0.1556
46	H	5.8638	2.9168	0.3834
47	C	-4.2804	-2.877	0.4046
48	H	-4.8059	-2.5975	-0.5199
49	C	-3.7671	-4.3283	0.2476
50	H	-3.1427	-4.439	-0.6454
51	H	-3.1785	-4.6342	1.1256
52	H	-4.6135	-5.0233	0.1568
53	C	-5.2618	-2.7765	1.5911
54	H	-5.5891	-1.7408	1.7272
55	H	-6.1424	-3.4118	1.4189
56	H	-4.7844	-3.1123	2.5246
57	O	-2.5501	-2.1174	-1.8069
58	O	2.5365	-0.1813	-2.9417
59	H	-0.4279	-1.858	0.6037
60	H	2.1205	-0.3059	0.258
61	C	3.2474	-0.6145	6.4838
62	C	3.6623	-1.9185	6.8368
63	C	4.4057	-2.1157	8.0177
64	C	4.7204	-1.0216	8.8469
65	C	4.298	0.2758	8.5013
66	C	3.5627	0.4749	7.3154
67	H	2.688	-0.4606	5.562
68	H	4.7554	-3.1112	8.2742
69	H	5.2972	-1.1833	9.7552
70	H	4.5429	1.1204	9.1422
71	H	3.24	1.4749	7.034
72	C	1.7995	-3.5689	6.0875
73	H	1.1708	-2.882	6.6526
74	H	1.3431	-3.8057	5.1249
75	O	1.9319	-4.8211	6.8804
76	C	3.2537	-5.245	6.877
77	O	3.6608	-6.2975	7.3541
78	O	4.0565	-4.2916	6.253
79	C	3.2699	-3.071	5.9265
80	H	3.4622	-2.8238	4.8806
81	I	1.3257	-1.4258	2.9061

- Lowest energy conformation for **[TS1]·**.

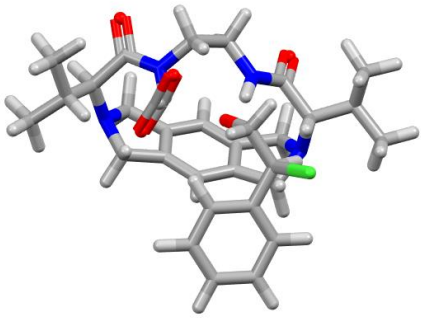


Cartesian coordinates (78 atoms). E (298.15 K) = -1626.120931 Hartree. Imaginary frequency: -253.2 *i* cm^{-1}

1	H	-0.0831	1.6108	2.686
2	C	-0.4621	1.6991	1.6716
3	C	-1.4044	1.8495	-1.0326
4	C	-1.6758	1.1171	1.2908
5	C	0.3025	2.3081	0.6654
6	C	-0.1583	2.3898	-0.663
7	C	-2.1432	1.1853	-0.0411
8	H	-1.7467	1.8767	-2.0651
9	C	1.7222	2.8434	0.7486
10	H	1.7467	3.8366	1.2269
11	H	2.3756	2.1962	1.3424
12	C	0.9303	3.0215	-1.5263
13	H	0.6902	4.0707	-1.7651
14	C	-2.6121	0.2128	2.0842
15	H	-2.0992	-0.4287	2.8076
16	H	-3.3616	0.8013	2.6375
17	C	-3.4103	0.33	-0.1456
18	H	-3.4932	-0.2274	-1.0812
19	H	-4.3141	0.9481	-0.0267
20	N	-3.3091	-0.5993	1.0333
21	C	-2.6905	-1.9519	0.7746
22	H	-2.0849	-2.1963	1.6591
23	C	-1.7629	-1.9738	-0.4703
24	N	-0.4245	-1.8124	-0.2732
25	C	0.4748	-1.7815	-1.4408
26	H	0.3479	-2.7155	-2.0066
27	H	0.1846	-0.9683	-2.118
28	C	1.9545	-1.6265	-1.0436
29	H	2.5644	-1.9115	-1.9064
30	H	2.1863	-2.2857	-0.2003
31	N	2.347	-0.2575	-0.6644
32	C	2.7929	0.6278	-1.6106
33	C	3.2366	2.0658	-1.1953
34	H	3.5469	2.4947	-2.1583
35	N	2.1647	2.9541	-0.6763
36	H	1.0823	2.4941	-2.4759
37	C	4.505	2.0455	-0.2912

38	H	4.251	1.5853	0.6752
39	C	5.6209	1.1896	-0.9363
40	H	6.5173	1.1972	-0.3013
41	H	5.3109	0.1473	-1.0739
42	H	5.8973	1.588	-1.9223
43	C	5.0147	3.4804	-0.0267
44	H	5.3011	3.9647	-0.9715
45	H	4.2449	4.1002	0.4425
46	H	5.8984	3.4602	0.6266
47	C	-3.792	-3.0445	0.6425
48	H	-4.3863	-2.7931	-0.2476
49	C	-3.1704	-4.4456	0.4293
50	H	-2.594	-4.4911	-0.501
51	H	-2.5079	-4.7121	1.2667
52	H	-3.9602	-5.2079	0.3767
53	C	-4.7127	-3.0461	1.8807
54	H	-5.1148	-2.0436	2.0574
55	H	-5.548	-3.747	1.7395
56	H	-4.1617	-3.3599	2.7804
57	O	-2.2492	-2.1261	-1.6377
58	O	2.8819	0.2967	-2.834
59	H	-0.0133	-1.6113	0.6533
60	H	2.1986	-0.0105	0.3124
61	Cl	0.6708	-2.1473	6.1769
62	C	1.7186	0.9258	5.1829
63	C	2.1217	0.0682	4.1324
64	C	3.3719	0.2925	3.5111
65	C	4.1983	1.3523	3.9261
66	C	3.785	2.2091	4.9647
67	C	2.5405	1.9895	5.5902
68	H	0.7953	0.7007	5.7083
69	H	3.6865	-0.351	2.6935
70	H	5.1595	1.5109	3.4404
71	H	4.424	3.0295	5.2858
72	H	2.2217	2.6339	6.4069
73	O	1.2675	-1.2217	1.9419
74	C	1.6593	-2.2189	2.9749
75	H	1.0186	-3.0982	3.0426
76	H	2.7237	-2.4655	2.9918
77	C	1.2191	-1.0296	3.709
78	H	0.1775	-0.9772	3.9829

- Lowest energy conformation for **[TS2]·**.

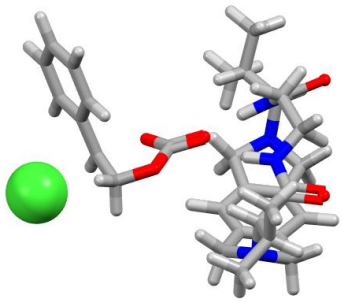


Cartesian coordinates (81 atoms). E (298.15 K) = -1814.675681 Hartree. Imaginary frequency: -23.9 *i* cm^{-1}

1	H	-0.7588	1.3164	2.8718
2	C	-1.0309	1.405	1.8202
3	C	-1.6842	1.4936	-0.9765
4	C	-2.1651	0.7619	1.3139
5	C	-0.2024	2.0562	0.9015
6	C	-0.518	2.1072	-0.4757
7	C	-2.4937	0.8025	-0.0589
8	H	-1.9081	1.4927	-2.0371
9	C	1.1779	2.6591	1.132
10	H	1.1097	3.6389	1.6349
11	H	1.8036	2.015	1.7696
12	C	0.6314	2.7588	-1.2322
13	H	0.3631	3.7786	-1.5709
14	C	-3.1283	-0.1914	2.0078
15	H	-2.6553	-0.7787	2.8001
16	H	-3.9758	0.3422	2.4501
17	C	-3.6779	-0.1454	-0.2958
18	H	-3.6107	-0.7029	-1.2305
19	H	-4.6262	0.4083	-0.2737
20	N	-3.6282	-1.0641	0.8906
21	C	-2.8438	-2.3459	0.7171
22	H	-2.3293	-2.5447	1.6662
23	C	-1.7568	-2.2689	-0.3981
24	N	-0.4591	-2.0803	-0.0325
25	C	0.5411	-2.0062	-1.1143
26	H	0.5668	-2.9685	-1.6469
27	H	0.2254	-1.2554	-1.8565
28	C	1.9477	-1.6921	-0.5867
29	H	2.6709	-1.9139	-1.3696
30	H	2.151	-2.306	0.2971
31	N	2.1523	-0.2717	-0.2151
32	C	2.8131	0.5927	-1.0446
33	C	2.9827	2.0938	-0.6277
34	H	3.3295	2.5555	-1.5652
35	N	1.7499	2.813	-0.2347
36	H	0.9206	2.1869	-2.1174

37	C	4.1429	2.2867	0.403
38	H	3.8351	1.87	1.3606
39	C	5.4238	1.5458	-0.0492
40	H	6.2314	1.7298	0.6788
41	H	5.2686	0.4561	-0.1109
42	H	5.7584	1.8842	-1.0352
43	C	4.4392	3.7967	0.5907
44	H	4.8029	4.2387	-0.3457
45	H	3.5391	4.3379	0.8909
46	H	5.2118	3.9349	1.3619
47	C	-3.8018	-3.542	0.4362
48	H	-4.3065	-3.3197	-0.5193
49	C	-3.0175	-4.862	0.2622
50	H	-2.3412	-4.8217	-0.5904
51	H	-2.4326	-5.0908	1.1606
52	H	-3.7146	-5.6962	0.1074
53	C	-4.8525	-3.6695	1.55
54	H	-5.3691	-2.7188	1.7025
55	H	-5.5933	-4.4428	1.3013
56	H	-4.3838	-3.9635	2.4982
57	O	-2.1071	-2.3708	-1.6256
58	O	3.3277	0.2112	-2.1454
59	H	-0.1142	-1.9646	0.9768
60	H	1.6756	0.0447	0.6253
61	C	-1.8369	-1.0054	5.8297
62	C	-0.6793	-1.2282	5.0626
63	C	0.3376	-0.2482	5.0563
64	C	0.2055	0.9249	5.8269
65	C	-0.9552	1.1326	6.5967
66	C	-1.9815	0.1665	6.5966
67	H	-2.6227	-1.7581	5.8499
68	H	1.1977	-0.3848	4.4138
69	H	0.9965	1.6723	5.8029
70	H	-1.0527	2.0445	7.1863
71	H	-2.8757	0.3282	7.1929
72	Cl	-0.591	-4.0296	5.5466
73	C	-0.5473	-2.5037	4.2591
74	H	-1.4601	-2.723	3.6857
75	C	0.7138	-2.7049	3.3844
76	H	1.5925	-2.6637	4.0576
77	H	0.6762	-3.7418	2.9955
78	O	0.751	-1.7209	2.3472
79	C	3.363	-1.1234	2.5945
80	O	3.1603	-0.0062	2.9755
81	O	3.7182	-2.2196	2.2704

- Lowest energy conformation for **[TS3]·**.

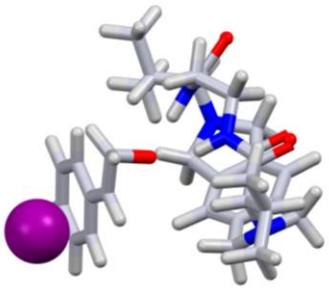


Cartesian coordinates (81 atoms). E (298.15 K) = -1814.699672 Hartree. Imaginary frequency: -282.0 *i* cm^{-1}

1	H	-0.1779	1.1037	2.9981
2	C	-0.5632	1.3026	2.001
3	C	-1.5217	1.7534	-0.6616
4	C	-1.7947	0.7929	1.5767
5	C	0.2158	1.9814	1.0521
6	C	-0.2546	2.213	-0.2545
7	C	-2.2708	1.0097	0.2639
8	H	-1.8715	1.8972	-1.6818
9	C	1.6627	2.4306	1.1667
10	H	1.7509	3.3567	1.759
11	H	2.2847	1.6788	1.6646
12	C	0.8492	2.8844	-1.0661
13	H	0.6483	3.9602	-1.1997
14	C	-2.7365	-0.1783	2.2797
15	H	-2.2184	-0.9034	2.9153
16	H	-3.4689	0.3563	2.9062
17	C	-3.5564	0.195	0.0841
18	H	-3.6614	-0.2558	-0.9051
19	H	-4.4464	0.8133	0.2809
20	N	-3.4604	-0.8579	1.1548
21	C	-2.8763	-2.1893	0.7485
22	H	-2.25	-2.5281	1.586
23	C	-1.9845	-2.109	-0.5201
24	N	-0.6376	-2.0087	-0.3419
25	C	0.249	-1.8889	-1.5132
26	H	0.0943	-2.7637	-2.1609
27	H	-0.0292	-1.0101	-2.108
28	C	1.7365	-1.8052	-1.1211
29	H	2.3291	-2.0156	-2.0168
30	H	1.9648	-2.5523	-0.3532
31	N	2.1639	-0.4915	-0.6115
32	C	2.6424	0.4713	-1.4574
33	C	3.1316	1.8365	-0.879
34	H	3.4482	2.37	-1.7862
35	N	2.0881	2.6839	-0.245
36	H	0.969	2.4455	-2.0642
37	C	4.4044	1.6699	0.004
38	H	4.1443	1.1037	0.9106

39	C	5.4886	0.8632	-0.7491
40	H	6.3873	0.767	-0.1251
41	H	5.1436	-0.1451	-1.0042
42	H	5.7716	1.3668	-1.6838
43	C	4.961	3.047	0.432
44	H	5.2657	3.6279	-0.4505
45	H	4.2109	3.6334	0.9711
46	H	5.8414	2.9206	1.0774
47	C	-4.0016	-3.2452	0.5419
48	H	-4.6114	-2.9017	-0.306
49	C	-3.4122	-4.6305	0.1832
50	H	-2.8613	-4.5986	-0.763
51	H	-2.7315	-4.9835	0.9726
52	H	-4.217	-5.372	0.0822
53	C	-4.8947	-3.3474	1.796
54	H	-5.279	-2.36	2.0709
55	H	-5.7426	-4.023	1.6129
56	H	-4.3276	-3.7463	2.6511
57	O	-2.5024	-2.13	-1.6828
58	O	2.7225	0.2762	-2.7107
59	H	-0.2149	-1.9127	0.5877
60	H	2.0368	-0.3487	0.3891
61	C	3.9835	-1.6312	6.4677
62	C	2.8088	-2.1802	5.9058
63	C	2.816	-3.5332	5.4964
64	C	3.9708	-4.3182	5.6505
65	C	5.1365	-3.7633	6.2128
66	C	5.1378	-2.4132	6.62
67	H	3.977	-0.5958	6.7988
68	H	1.9262	-3.9715	5.0519
69	H	3.9632	-5.3584	5.3317
70	H	6.0303	-4.3724	6.3329
71	H	6.033	-1.9794	7.0605
72	Cl	0.7908	-1.4773	8.1359
73	C	1.6187	-1.3151	5.7184
74	H	1.6756	-0.2993	6.0725
75	C	0.2529	-1.8805	5.3306
76	H	0.0505	-2.8284	5.8243
77	H	-0.5352	-1.1665	5.5724
78	O	0.1975	-2.1614	3.8615
79	C	1.1476	-1.4197	3.1425
80	O	1.1352	-1.4835	1.8848
81	O	1.956	-0.7193	3.9066

- Lowest energy conformation for **[TS1(I)]·**.

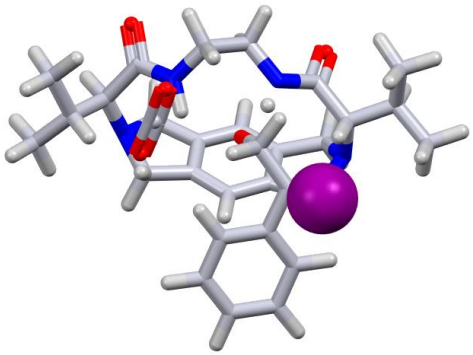


Cartesian coordinates (78 atoms). E (298.15 K) = -1622.574526 Hartree. Imaginary frequency: -226.5 *i* cm^{-1}

1	H	-0.0853	1.5625	2.7006
2	C	-0.4707	1.6758	1.6915
3	C	-1.4175	1.8651	-1.0082
4	C	-1.6908	1.111	1.3075
5	C	0.297	2.2898	0.6914
6	C	-0.1659	2.3903	-0.6351
7	C	-2.1608	1.197	-0.0223
8	H	-1.7605	1.9051	-2.04
9	C	1.7232	2.8053	0.7781
10	H	1.7629	3.7907	1.2711
11	H	2.3687	2.1396	1.3602
12	C	0.9292	3.0166	-1.4943
13	H	0.7005	4.0699	-1.7261
14	C	-2.6289	0.2035	2.0936
15	H	-2.1124	-0.4509	2.8031
16	H	-3.3713	0.7889	2.6601
17	C	-3.4333	0.3503	-0.1332
18	H	-3.52	-0.1983	-1.0737
19	H	-4.3336	0.9722	-0.0084
20	N	-3.337	-0.5911	1.0372
21	C	-2.732	-1.9471	0.7645
22	H	-2.1275	-2.2057	1.6457
23	C	-1.8049	-1.965	-0.4805
24	N	-0.4653	-1.8119	-0.2831
25	C	0.4309	-1.7801	-1.4535
26	H	0.2934	-2.7092	-2.0246
27	H	0.1449	-0.96	-2.1241
28	C	1.9132	-1.6393	-1.0624
29	H	2.517	-1.9167	-1.9317
30	H	2.1459	-2.313	-0.2307
31	N	2.3149	-0.2774	-0.668
32	C	2.7784	0.6092	-1.6042
33	C	3.2295	2.041	-1.1762
34	H	3.5407	2.4777	-2.1353
35	N	2.1633	2.9291	-0.646
36	H	1.0743	2.494	-2.4477
37	C	4.4992	2.0049	-0.2742

38	H	4.2431	1.5385	0.6887
39	C	5.6087	1.1466	-0.9271
40	H	6.5065	1.1453	-0.294
41	H	5.2924	0.1069	-1.07
42	H	5.8851	1.5488	-1.9114
43	C	5.0187	3.4344	0.0006
44	H	5.3108	3.9226	-0.9404
45	H	4.2519	4.0567	0.4717
46	H	5.9008	3.4038	0.6556
47	C	-3.8436	-3.0278	0.622
48	H	-4.4361	-2.7619	-0.2651
49	C	-3.236	-4.4326	0.3943
50	H	-2.6627	-4.4749	-0.538
51	H	-2.5735	-4.7136	1.2269
52	H	-4.0331	-5.1868	0.3366
53	C	-4.7642	-3.033	1.8604
54	H	-5.1551	-2.0281	2.0485
55	H	-5.6072	-3.7228	1.7114
56	H	-4.2168	-3.3642	2.7563
57	O	-2.2925	-2.107	-1.6484
58	O	2.8787	0.285	-2.8287
59	H	-0.0545	-1.6094	0.6431
60	H	2.1498	-0.0393	0.31
61	C	1.6615	1.0245	5.0328
62	C	2.2207	0.0678	4.1515
63	C	3.5243	0.2924	3.6474
64	C	4.2443	1.4415	4.0134
65	C	3.6769	2.388	4.89
66	C	2.3807	2.172	5.4
67	H	0.6785	0.8376	5.4583
68	H	3.9746	-0.4317	2.974
69	H	5.2475	1.5981	3.6221
70	H	4.2375	3.2748	5.1765
71	H	1.9401	2.8897	6.0887
72	O	1.2266	-1.1688	1.9282
73	C	1.843	-2.157	2.8361
74	H	1.3123	-3.1072	2.9204
75	H	2.917	-2.3061	2.6929
76	C	1.4188	-1.1095	3.7752
77	H	0.4074	-1.1755	4.1508
78	I	1.5772	-2.7573	6.4298

- Lowest energy conformation for **[TS2(I)]·**.

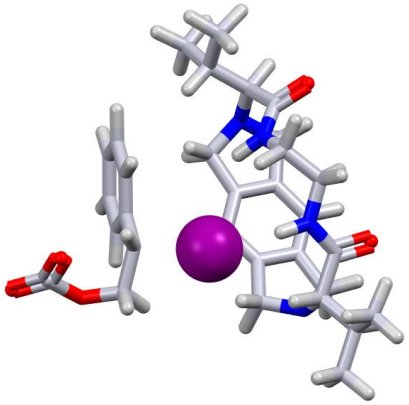


Cartesian coordinates (81 atoms). E (298.15 K) = -1811.117787 Hartree. Imaginary frequency: -21.0 *i* cm^{-1}

1	H	-0.7975	1.2426	2.8935
2	C	-1.0701	1.3532	1.8479
3	C	-1.7099	1.4955	-0.946
4	C	-2.2007	0.7195	1.3242
5	C	-0.236	2.0261	0.9417
6	C	-0.5483	2.1003	-0.4297
7	C	-2.5182	0.7788	-0.0514
8	H	-1.9254	1.5084	-2.0124
9	C	1.1385	2.6239	1.1924
10	H	1.0672	3.5948	1.7112
11	H	1.7575	1.9769	1.8251
12	C	0.6005	2.7726	-1.172
13	H	0.3355	3.7939	-1.4912
14	C	-3.1589	-0.2536	1.9951
15	H	-2.6846	-0.8558	2.7727
16	H	-4.0121	0.2752	2.4513
17	C	-3.6993	-0.1632	-0.3078
18	H	-3.63	-0.7097	-1.256
19	H	-4.6552	0.3841	-0.2837
20	N	-3.6617	-1.1054	0.8669
21	C	-2.8789	-2.3845	0.6693
22	H	-2.3735	-2.5931	1.622
23	C	-1.7944	-2.2924	-0.4371
24	N	-0.5058	-2.103	-0.0578
25	C	0.5173	-2.0063	-1.1148
26	H	0.5546	-2.9571	-1.6691
27	H	0.2277	-1.2401	-1.8459
28	C	1.9165	-1.7063	-0.5513
29	H	2.6588	-1.9293	-1.3222
30	H	2.0975	-2.3301	0.3278
31	N	2.1198	-0.2947	-0.1616
32	C	2.7713	0.5848	-0.994
33	C	2.9456	2.0819	-0.5717
34	H	3.2881	2.5398	-1.513
35	N	1.7179	2.8061	-0.1738
36	H	0.8984	2.2151	-2.0684

37	C	4.1085	2.2711	0.4522
38	H	3.8021	1.8524	1.426
39	C	5.3859	1.5241	0.0026
40	H	6.1983	1.7087	0.7192
41	H	5.2297	0.4416	-0.0667
42	H	5.7144	1.8685	-0.9872
43	C	4.4089	3.7752	0.648
44	H	4.7728	4.2195	-0.289
45	H	3.5105	4.3234	0.949
46	H	5.185	3.9166	1.413
47	C	-3.8449	-3.5697	0.373
48	H	-4.3518	-3.3376	-0.574
49	C	-3.0697	-4.8967	0.193
50	H	-2.3877	-4.846	-0.662
51	H	-2.4831	-5.1348	1.093
52	H	-3.7693	-5.7274	0.022
53	C	-4.9017	-3.7098	1.489
54	H	-5.4146	-2.7557	1.647
55	H	-5.6442	-4.4769	1.225
56	H	-4.432	-4.0135	2.437
57	O	-2.1346	-2.3973	-1.666
58	O	3.2717	0.2129	-2.096
59	H	-0.1815	-1.9744	0.953
60	H	1.645	0.0039	0.686
61	C	-1.878	-0.8086	5.61
62	C	-0.6272	-1.1706	5.055
63	C	0.4667	-0.2937	5.235
64	C	0.316	0.8987	5.966
65	C	-0.9305	1.2418	6.526
66	C	-2.0314	0.3815	6.341
67	H	-2.7286	-1.4761	5.483
68	H	1.4202	-0.5247	4.777
69	H	1.1684	1.5641	6.087
70	H	-1.0443	2.1658	7.089
71	H	-3.0018	0.638	6.761
72	C	-0.4934	-2.4579	4.29
73	H	-1.4227	-2.7319	3.785
74	C	0.7211	-2.6564	3.365
75	H	1.6441	-2.5813	3.976
76	H	0.6916	-3.696	2.986
77	O	0.6388	-1.6774	2.337
78	C	3.5225	-1.1487	2.627
79	O	3.2986	-0.0668	3.083
80	O	3.8509	-2.2151	2.207
81	I	-0.458	-4.2392	5.868

- Lowest energy conformation for **[TS3(I)]·**.



Cartesian coordinates (81 atoms). E (298.15 K) = -1811.122363 Hartree. Imaginary frequency: -53.0 *i* cm^{-1}

1	H	-0.0505	0.6052	3.3033
2	C	-0.4549	0.9533	2.3554
3	C	-1.482	1.8155	-0.1798
4	C	-1.6766	0.4749	1.8625
5	C	0.2697	1.8332	1.535
6	C	-0.2256	2.2443	0.2808
7	C	-2.1942	0.9114	0.6231
8	H	-1.8569	2.1126	-1.1566
9	C	1.6718	2.3994	1.7276
10	H	1.6468	3.281	2.3893
11	H	2.371	1.6913	2.185
12	C	0.8422	3.0733	-0.427
13	H	0.5977	4.1465	-0.4017
14	C	-2.5893	-0.6163	2.4115
15	H	-2.0477	-1.4497	2.8714
16	H	-3.281	-0.2135	3.1683
17	C	-3.4914	0.1489	0.346
18	H	-3.6205	-0.1268	-0.7028
19	H	-4.3661	0.7363	0.666
20	N	-3.3798	-1.0694	1.2194
21	C	-2.8634	-2.3084	0.5444
22	H	-2.3981	-2.9178	1.3324
23	C	-1.7977	-2.0097	-0.5503
24	N	-0.4789	-2.1411	-0.1994
25	C	0.5982	-1.9283	-1.1846
26	H	0.6774	-2.8164	-1.8303
27	H	0.3215	-1.093	-1.8322
28	C	1.978	-1.6783	-0.5409
29	H	2.736	-1.9075	-1.2969
30	H	2.1293	-2.3503	0.3132
31	N	2.2305	-0.3003	-0.0876
32	C	2.7441	0.6512	-0.9371
33	C	3.1453	2.0458	-0.3608
34	H	3.3828	2.6188	-1.2668
35	N	2.0945	2.8129	0.3535

36	H	0.9728	2.7896	-1.4777
37	C	4.4688	1.9467	0.4637
38	H	4.2667	1.3896	1.3903
39	C	5.5611	1.1735	-0.3109
40	H	6.4964	1.1724	0.2658
41	H	5.2764	0.1311	-0.4959
42	H	5.7586	1.6409	-1.2845
43	C	4.9735	3.3571	0.8413
44	H	5.248	3.918	-0.0665
45	H	4.2	3.9329	1.3671
46	H	5.866	3.2872	1.4811
47	C	-4.0309	-3.1391	-0.0645
48	H	-4.4959	-2.5208	-0.8457
49	C	-3.5083	-4.4348	-0.7279
50	H	-2.8304	-4.2161	-1.5588
51	H	-2.978	-5.0632	0.0013
52	H	-4.347	-5.0235	-1.1238
53	C	-5.0873	-3.4699	1.0103
54	H	-5.4234	-2.558	1.5119
55	H	-5.9549	-3.97	0.5575
56	H	-4.6722	-4.1456	1.7726
57	O	-2.1389	-1.646	-1.7162
58	O	2.953	0.397	-2.159
59	H	-0.2319	-2.4726	0.731
60	H	1.9878	-0.0555	0.8644
61	C	3.7442	-1.8749	4.3621
62	C	2.4682	-1.9644	4.9699
63	C	1.8405	-0.774	5.4139
64	C	2.4686	0.4704	5.2338
65	C	3.7314	0.5485	4.6131
66	C	4.3712	-0.6328	4.1813
67	H	4.2413	-2.7878	4.0394
68	H	0.8979	-0.8329	5.9468
69	H	1.9865	1.3753	5.5992
70	H	4.221	1.5132	4.4881
71	H	5.3564	-0.5835	3.7207
72	C	1.8469	-3.3036	5.1586
73	H	2.5583	-4.1194	5.1917
74	C	0.6765	-3.4702	6.1426
75	H	-0.2235	-2.9634	5.7748
76	H	0.469	-4.5431	6.2437
77	O	0.9459	-2.8615	7.4325
78	C	2.1707	-3.3867	8.1488
79	O	2.2761	-2.9442	9.3158
80	O	2.8795	-4.1771	7.4257
81	I	0.8432	-3.9936	3.0109