

Anexo VI:

Computational methods

Capítulo 4:

Alkenylarenes as dipolarophiles in catalytic asymmetric 1,3-dipolar cycloadditions of azomethine ylides..... 2

Capítulo 4: Alkenylarenes as dipolarophiles in catalytic asymmetric 1,3-dipolar cycloadditions of azomethine ylides

Hybrid QM/MM calculations for optimization of saddle points were performed using the ONIOM¹ method as implemented in Gaussian09 suite of programs. Atoms within the high layer are gathered in ball & stick representation. Transparent stick model atoms represent the ones included in the low layer. In the high level layer, the electron correlation was taken into account by using the hybrid functional B3LYP together with the Hay-Wadt core effective potential (ECP) and basis set.² PM6³ semiempirical Hamiltonian was employed in the low level layer. In order to describe properly nonbonding interactions and dispersion forces, single-point calculations on the optimized ONIOM structures were carried out employing the Minnesota functional M06L (see ref. 13f of the main text). Thermal corrections were computed at same level of theory used in the optimization and were not scaled. All stationary points were characterized by harmonic analysis. Reactants, intermediates and cycloadducts have positive definite Hessian matrices. Transition structures show only one negative eigenvalue in their diagonalized force constant matrices, and their associated eigenvectors were confirmed to correspond to the motion along the reaction coordinate under study. Figures including optimized structures were made with the Maestro interface.⁴

Fukui functions associated with electrophilic or nucleophilic attacks (f^+ and f^- respectively) were computed according to equations E1 and E2,⁵ in which the terms on the right part of the equations correspond to the NBO charge of atom i with $N+1$, N or $N-1$ electrons, respectively.

$$f^+ = q_i(N+1) - q_i(N) \quad (\text{E1})$$

$$f^- = q_i(N) - q_i(N-1) \quad (\text{E2})$$

¹. S. Dapprich, I. Komáromi, K. S. Byun, K. Morokuma, M. J. Frisch *J. Mol. Struct. (Theochem)* **1999**, *462*, 1-21.

². P. J. Hay, W. R. Wadt, *J. Chem. Phys.*, **1985**, *82*, 299-303.

³. J. J. P. Stewart, *J. Mol. Model.*, **2007**, *13*, 1173-1213.

⁴. Maestro, version 9.2, Schrödinger LLC, New York, 2013.

⁵. W. Yang, W. J. Mortier, *J. Am. Chem. Soc.* **1986**, *108*, 5708-5711.

Additional TS associated with the studied cycloadditions

Figures VI.1 – VI.3 include the main geometrical features and relative energies (referred to the less energetic transition structure) associated with the studied cycloadditions.

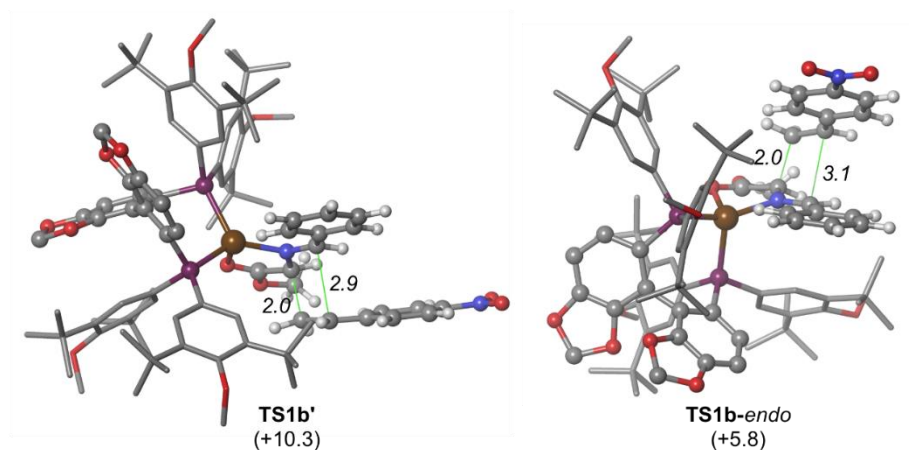


Figure VI.1. Main geometric features and relative energies (in kcal mol⁻¹) of additional transition structures associated with the dipolar cycloaddition of *p*-nitrostyrene **59a** with the azomethine ylide derived from imine **48a** Cu(I) and chiral ligand (*R*)-DTBM-Segphos computed at the M06L/LANL2DZ//ONIOM-(B3LYP/LANL2DZ:PM6) level of theory. Distances are in Å.

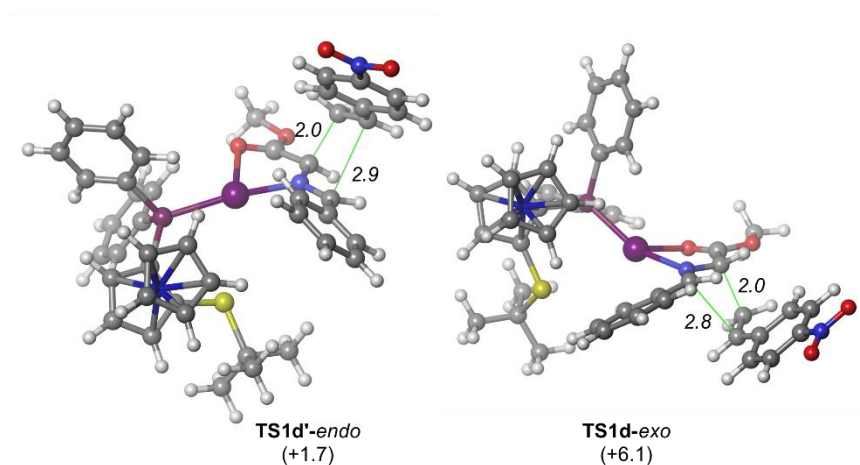


Figure VI.2. Main geometric features and relative energies (in kcal mol⁻¹) of additional transition structures associated with the dipolar cycloaddition of *p*-nitrostyrene **59a** with the azomethine ylide derived from imine **48a** Ag(I) and chiral ligand (*R*)-Fesulphos computed at the M06L/LANL2DZ//ONIOM-(B3LYP/LANL2DZ:PM6) level of theory. Distances are in Å.

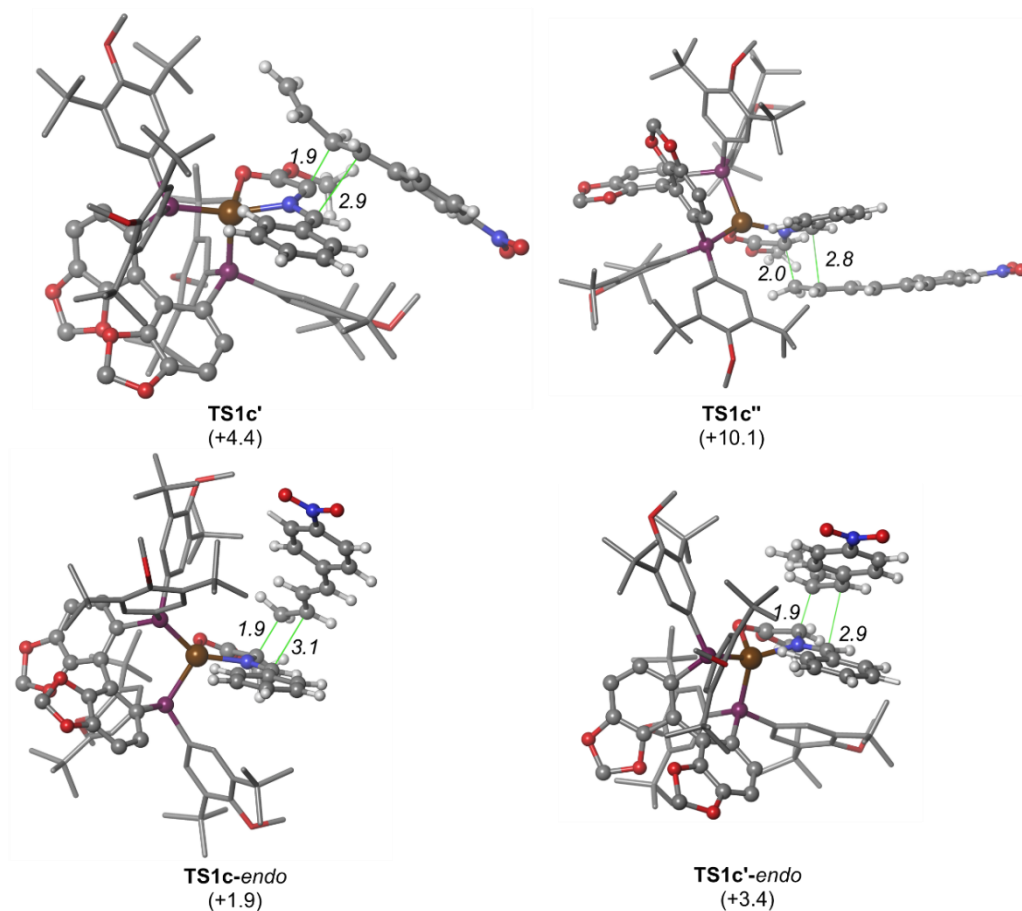


Figure VI.3. Main geometric features and relative energies (in kcal mol⁻¹) of additional transition structures associated with the dipolar cycloaddition of *p*-nitrophenyl-1,3-butadiene **61c** with the azomethine ylide derived from imine **48a** Cu(I) and chiral ligand (*R*)-DTBM-Segphos computed at the M06L/LANL2DZ//ONIOM-(B3LYP/LANL2DZ:PM6) level of theory. Distances are in Å.

Table VI.1. Total electronic energies^a (E, in a.u.), thermal corrections to Gibbs free energies^b (TCGFE, in a.u.), and number of imaginary frequencies^c (NIMAG) of all stationary points discussed in the main text corresponding to the dipolar cycloaddition of styrene **59m** or *p*-nitrostyrene **59a** with azomethine ylide derived from imine **48a** and Cu/(*R*)-DTBM-Segphos as catalytic system.

Structure	E	TCGFE	NIMAG(ν)
48a	-592.687098	0.151773	0
59m	-309.557617	0.103468	0
59a	-514.017615	0.101028	0
INT1a	-4282.123612	1.499817	0
INT2b	-4796.143355	1.623268	0
INT2a	-4591.676963	1.625655	0
INT3b	-4796.140667	1.622599	0
<i>exo</i> - 64m	-902.295028	0.287585	0
<i>exo</i> - 64a	-1106.755080	0.284471	0
ET1a	-4591.665845	1.627758	1 (-137.3453)
ET1b	-4796.140511	1.621820	1 (-355.8175)
ET1b'	-4796.127380	1.625111	1 (-358.8138)
ET1b-endo	-4796.141307	1.631849	1 (-362.0074)
ET2b	-4796.128142	1.623431	1 (-241.2497)

^aComputed at M06L/LANL2DZ//ONIOM(B3LYP/LANL2DZ:PM6) level of theory. ^bComputed at 298.15 K ONIOM(B3LYP/LANL2DZ:PM6) level of theory. ^cIf NIMAG=1, the imaginary frequency ν (in parentheses) is given in cm^{-1} .

Cartesian of all the stationary collected in Table VI.1.

48a

Center	Atomic	Atomic	Coordinates (Angstroms)
--------	--------	--------	-------------------------

Number	Number	Type	X	Y	Z
1	7	0	0.603695	0.480628	-0.488138
2	6	0	-0.319101	-0.424008	-0.578817
3	6	0	1.988471	0.107745	-0.787550
4	1	0	-0.093195	-1.456281	-0.896046
5	6	0	-1.735287	-0.149630	-0.269477
6	6	0	-2.689283	-1.181659	-0.421968
7	6	0	-2.157658	1.125371	0.178826
8	6	0	-4.045882	-0.946937	-0.134889
9	1	0	-2.368167	-2.165797	-0.760104
10	6	0	-3.510976	1.358356	0.464321
11	1	0	-1.411548	1.905460	0.297426
12	6	0	-4.459328	0.323891	0.308049
13	1	0	-4.773255	-1.746325	-0.252791
14	1	0	-3.831711	2.338025	0.810481
15	1	0	-5.507457	0.507786	0.532506
16	1	0	2.483857	0.968066	-1.245010
17	6	0	2.729298	-0.334483	0.494406
18	8	0	2.176843	-0.925507	1.423265
19	8	0	4.099559	-0.109991	0.564054
20	6	0	4.840905	0.614253	-0.475825
21	1	0	4.546434	1.670008	-0.505345
22	1	0	5.886764	0.534166	-0.174681
23	1	0	4.708405	0.153572	-1.462204
24	1	0	2.075841	-0.746481	-1.488271

59m

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

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-----
  1      6      0    -0.693614  -1.788126  -0.000000
  2      6      0     0.654978  -2.202028  -0.000000
  3      6      0     1.676269  -1.233608   0.000000
  4      6      0     1.349277   0.133767   0.000000
  5      6      0     0.000000   0.564786   0.000000
  6      6      0    -1.017798  -0.422504  -0.000000
  7      6      0    -0.280803   2.017488   0.000000
  8      6      0    -1.491487   2.622294  -0.000000
  9      1      0     0.902577  -3.260902  -0.000000
 10      1      0     2.719272  -1.541614   0.000000
 11      1      0     2.143874   0.878245   0.000000
 12      1      0    -2.063095  -0.123740  -0.000000
 13      1      0    -1.487581  -2.531592  -0.000000
 14      1      0     0.606096   2.654164   0.000000
 15      1      0    -1.575155   3.705771   0.000000
 16      1      0    -2.426926   2.067254  -0.000000
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59b

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Center   Atomic   Atomic          Coordinates (Angstroms)
Number   Number   Type            X           Y           Z
-----
  1      6      0    -0.000000  -1.085782  -0.000000
  2      7      0     0.132926  -2.551894  -0.000000
  3      6      0    -1.284201  -0.514831   0.000000
  4      6      0    -1.395138   0.881224   0.000000
  5      6      0    -0.247539   1.714420   0.000000
  6      6      0     1.032354   1.099456  -0.000000
  7      6      0     1.163749  -0.292389  -0.000000
  8      1      0    -2.157262  -1.157611   0.000000
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9	1	0	-2.382329	1.337264	0.000000
10	6	0	-0.438310	3.179217	0.000000
11	1	0	1.928711	1.712086	-0.000000
12	1	0	2.135831	-0.772678	-0.000000
13	6	0	0.528432	4.126242	0.000000
14	1	0	-1.478018	3.508545	0.000000
15	1	0	0.273963	5.182506	0.000000
16	1	0	1.589907	3.888883	0.000000
17	8	0	1.311794	-3.053125	-0.000000
18	8	0	-0.936465	-3.257011	-0.000000

INT1a

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-0.164379	-2.059603	-2.959331
2	6	0	0.267745	-1.062365	-2.082829
3	6	0	1.224468	-1.475590	-1.100148
4	6	0	1.643936	-2.819815	-1.025042
5	6	0	1.168819	-3.811441	-1.917337
6	6	0	0.263431	-3.392757	-2.879386
7	1	0	2.362808	-3.115996	-0.263572
8	1	0	1.503953	-4.840044	-1.857501
9	6	0	-0.221813	0.343225	-2.278171
10	6	0	-1.197886	1.006469	-1.460381
11	6	0	0.230796	1.061360	-3.385581
12	6	0	-1.640177	2.302322	-1.790320
13	6	0	-0.216839	2.352566	-3.699727
14	6	0	-1.157645	3.005380	-2.920645
15	1	0	-2.382753	2.793138	-1.166826

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16	1	0	-1.511127	4.000049	-3.164339
17	8	0	-1.048750	-1.905070	-4.047932
18	8	0	-0.323489	-4.160298	-3.905088
19	8	0	0.383741	2.802541	-4.892695
20	8	0	1.154318	0.622729	-4.361596
21	6	0	-1.279975	-3.262944	-4.583551
22	6	0	1.407810	1.793645	-5.226499
23	1	0	2.408958	2.205108	-5.001148
24	1	0	1.291497	1.496997	-6.269710
25	1	0	-2.311968	-3.576244	-4.344841
26	1	0	-1.071663	-3.262046	-5.654871
27	15	0	1.819876	-0.244864	0.206422
28	15	0	-1.834252	0.145709	0.113642
29	29	0	0.017348	0.218894	1.618824
30	6	0	3.397723	-1.036893	0.801811
31	6	0	3.586704	-1.225697	2.166441
32	6	0	4.393945	-1.399980	-0.105412
33	6	0	4.800991	-1.739065	2.661257
34	1	0	2.796901	-0.973373	2.887694
35	6	0	5.633374	-1.883963	0.327674
36	1	0	4.220289	-1.292172	-1.184847
37	6	0	5.831162	-1.976022	1.726858
38	6	0	2.505788	1.172330	-0.767467
39	6	0	2.161583	2.465509	-0.392388
40	6	0	3.373144	0.951861	-1.838259
41	6	0	2.713883	3.577287	-1.056389
42	1	0	1.447654	2.655842	0.434355
43	6	0	4.006116	2.016714	-2.489108
44	1	0	3.579802	-0.073351	-2.170215
45	6	0	3.697071	3.322112	-2.033627
46	6	0	-3.259950	1.224074	0.641711
47	6	0	-4.582794	0.802956	0.526072

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48	6	0	-2.967229	2.466075	1.205492
49	6	0	-5.643182	1.601202	0.984523
50	1	0	-4.827878	-0.170964	0.087857
51	6	0	-3.986244	3.315617	1.663535
52	1	0	-1.917597	2.801952	1.317435
53	6	0	-5.308811	2.822321	1.610760
54	6	0	-2.767224	-1.300166	-0.611170
55	6	0	-2.873967	-2.486861	0.105505
56	6	0	-3.397675	-1.154519	-1.848035
57	6	0	-3.666109	-3.546688	-0.374481
58	1	0	-2.352739	-2.615351	1.061391
59	6	0	-4.211365	-2.170764	-2.367348
60	1	0	-3.271958	-0.232712	-2.427975
61	6	0	-4.382674	-3.327180	-1.570542
62	7	0	0.061790	0.176656	3.714307
63	6	0	0.096896	-0.830051	4.570322
64	6	0	0.038690	1.493580	4.166949
65	6	0	0.181840	-2.253542	4.245681
66	6	0	0.227462	-3.179852	5.324808
67	6	0	0.255714	-2.775896	2.926379
68	6	0	0.355340	-4.559252	5.099295
69	1	0	0.167868	-2.804404	6.345386
70	6	0	0.395926	-4.153736	2.702738
71	1	0	0.210083	-2.096880	2.076812
72	6	0	0.447262	-5.057883	3.784380
73	1	0	0.388439	-5.243855	5.944270
74	1	0	0.464063	-4.526041	1.681270
75	1	0	0.555416	-6.125233	3.605323
76	6	0	-3.715539	-4.855156	0.427619
77	6	0	-4.909307	-4.781318	1.400285
78	1	0	-5.859744	-4.651182	0.862375
79	1	0	-4.991217	-5.696114	1.995607

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80	1	0	-4.804984	-3.942623	2.096378
81	6	0	-3.836896	-6.081603	-0.493365
82	1	0	-4.796192	-6.110813	-1.023979
83	1	0	-3.056990	-6.074648	-1.262926
84	1	0	-3.745878	-7.015161	0.068744
85	6	0	-2.421094	-5.044902	1.249050
86	1	0	-1.540050	-5.065634	0.598948
87	1	0	-2.273634	-4.249882	1.990944
88	1	0	-2.441266	-5.989012	1.803432
89	6	0	-4.872562	-1.970862	-3.738539
90	6	0	-4.117322	-0.916882	-4.578977
91	1	0	-4.198665	0.088547	-4.150941
92	1	0	-3.046359	-1.146987	-4.656939
93	1	0	-4.517535	-0.861580	-5.595800
94	6	0	-4.870655	-3.284086	-4.542007
95	1	0	-5.509821	-4.047700	-4.076315
96	1	0	-5.230121	-3.133925	-5.563053
97	1	0	-3.859454	-3.714083	-4.591410
98	6	0	-6.313580	-1.468632	-3.522746
99	1	0	-6.823831	-1.308113	-4.477483
100	1	0	-6.911893	-2.189593	-2.946828
101	1	0	-6.327109	-0.518879	-2.975115
102	6	0	5.006091	1.713779	-3.612108
103	6	0	2.210387	4.974487	-0.664548
104	6	0	3.117994	5.520168	0.456086
105	1	0	3.068001	4.883862	1.346987
106	1	0	4.168482	5.570545	0.137420
107	1	0	2.811951	6.526937	0.755907
108	6	0	0.761515	4.898179	-0.136901
109	1	0	0.077895	4.511445	-0.899526
110	1	0	0.666516	4.235367	0.744066
111	1	0	0.398993	5.882151	0.172072

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112	6	0	2.200710	5.929073	-1.871504
113	1	0	1.652070	5.491195	-2.713021
114	1	0	1.726621	6.881978	-1.621447
115	1	0	3.210177	6.147437	-2.237686
116	6	0	6.428174	1.747257	-3.017696
117	1	0	7.184259	1.561952	-3.785921
118	1	0	6.649225	2.724439	-2.563294
119	1	0	6.554319	0.983111	-2.232479
120	6	0	4.876054	2.732852	-4.757972
121	1	0	5.144831	3.748249	-4.431331
122	1	0	5.519124	2.479015	-5.603828
123	1	0	3.837610	2.789712	-5.117482
124	6	0	4.768887	0.310884	-4.219968
125	1	0	5.033743	-0.496078	-3.517726
126	1	0	3.721320	0.167912	-4.512029
127	1	0	5.383165	0.161630	-5.113365
128	6	0	6.692880	-2.253402	-0.719745
129	6	0	7.630433	-1.044094	-0.906540
130	1	0	7.085679	-0.171122	-1.303859
131	1	0	8.090766	-0.741151	0.045307
132	1	0	8.440434	-1.274676	-1.604707
133	6	0	6.047395	-2.578802	-2.088148
134	1	0	5.297810	-3.371566	-1.998416
135	1	0	5.565446	-1.700377	-2.546852
136	1	0	6.803406	-2.928024	-2.799668
137	6	0	7.485738	-3.499656	-0.291533
138	1	0	8.189668	-3.816772	-1.065296
139	1	0	8.063405	-3.322510	0.626356
140	1	0	6.816498	-4.339993	-0.078688
141	6	0	4.931040	-1.992323	4.170691
142	6	0	3.548905	-2.259203	4.804938
143	1	0	2.870546	-1.400841	4.714071

144	1	0	3.048152	-3.117503	4.339437
145	1	0	3.640015	-2.479311	5.872853
146	6	0	5.801303	-3.227285	4.461885
147	1	0	5.431053	-4.105155	3.921287
148	1	0	6.843220	-3.084674	4.149998
149	1	0	5.807719	-3.468901	5.528289
150	6	0	5.536507	-0.732041	4.820828
151	1	0	6.528714	-0.501767	4.406461
152	1	0	4.898787	0.143505	4.658894
153	1	0	5.652265	-0.861865	5.901111
154	8	0	7.087123	-2.396387	2.191522
155	8	0	-5.245263	-4.330673	-2.039838
156	8	0	-6.347213	3.607802	2.137615
157	8	0	4.352004	4.402258	-2.647305
158	6	0	5.516119	4.867624	-1.919597
159	1	0	6.278092	4.073803	-1.897340
160	1	0	5.845265	5.721127	-2.520967
161	1	0	5.229388	5.181470	-0.903164
162	6	0	-6.609844	3.359231	3.541416
163	1	0	-7.408304	4.074460	3.762641
164	1	0	-6.950485	2.321427	3.678016
165	1	0	-5.707419	3.568845	4.137497
166	6	0	-3.602119	4.702954	2.199441
167	6	0	-2.270953	5.182618	1.580649
168	1	0	-1.425144	4.532327	1.868740
169	1	0	-2.316732	5.209841	0.489115
170	1	0	-2.014423	6.187551	1.928039
171	6	0	-4.668657	5.755297	1.847813
172	1	0	-5.623314	5.560291	2.351644
173	1	0	-4.345813	6.760471	2.131428
174	1	0	-4.877895	5.759451	0.773162
175	6	0	-3.416890	4.597356	3.726353

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176	1	0	-3.192986	5.573744	4.164715
177	1	0	-4.317093	4.204979	4.218950
178	1	0	-2.580712	3.927782	3.968131
179	6	0	-7.082036	1.101705	0.796355
180	6	0	-7.176064	0.091458	-0.372721
181	1	0	-6.844869	0.543790	-1.314934
182	1	0	-6.563485	-0.800399	-0.197919
183	1	0	-8.207824	-0.243882	-0.514455
184	6	0	-8.038548	2.258782	0.460945
185	1	0	-8.121604	2.974907	1.290265
186	1	0	-7.680822	2.828919	-0.402897
187	1	0	-9.045385	1.898487	0.236284
188	6	0	-7.520845	0.388044	2.090835
189	1	0	-8.545857	0.015105	2.012651
190	1	0	-6.869081	-0.461469	2.317494
191	1	0	-7.483027	1.070122	2.953954
192	6	0	-6.599040	-4.225600	-1.532122
193	1	0	-7.087199	-5.096676	-1.981645
194	1	0	-6.598690	-4.290545	-0.432919
195	1	0	-7.055533	-3.286740	-1.881632
196	6	0	7.992608	-1.305523	2.494493
197	1	0	8.886915	-1.832255	2.843293
198	1	0	8.198718	-0.727122	1.580848
199	1	0	7.566854	-0.670800	3.287506
200	6	0	0.012625	2.533354	3.221291
201	8	0	-0.004917	2.364068	1.936046
202	8	0	-0.005931	3.877231	3.624403
203	6	0	0.089339	4.219371	5.040456
204	1	0	1.023704	3.842169	5.478812
205	1	0	0.081263	5.311569	5.071841
206	1	0	-0.767548	3.828145	5.606843
207	1	0	0.043371	1.680037	5.237309

208 1 0 0.080919 -0.600009 5.642905

INT2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.317332	2.209989	-3.637027
2	6	0	-0.831326	1.974958	-2.348713
3	6	0	0.457032	1.345644	-2.289872
4	6	0	1.126022	0.961895	-3.469519
5	6	0	0.587528	1.192436	-4.758090
6	6	0	-0.635958	1.840346	-4.804342
7	1	0	2.109887	0.502530	-3.405109
8	1	0	1.119911	0.904858	-5.656615
9	6	0	-1.590312	2.591077	-1.201605
10	6	0	-2.366210	1.945334	-0.175513
11	6	0	-1.625910	3.989346	-1.182786
12	6	0	-3.100417	2.720882	0.749171
13	6	0	-2.349119	4.742864	-0.247327
14	6	0	-3.110324	4.135379	0.735715
15	1	0	-3.683896	2.223628	1.521174
16	1	0	-3.682848	4.706653	1.455872
17	8	0	-2.525879	2.862081	-3.980427
18	8	0	-1.372068	2.237064	-5.942688
19	8	0	-2.208172	6.117585	-0.505673
20	8	0	-0.983424	4.857417	-2.094428
21	6	0	-2.395688	3.161634	-5.420398
22	6	0	-1.183715	6.221663	-1.563699
23	1	0	-0.238222	6.585608	-1.122280
24	1	0	-1.558531	6.863374	-2.361552

Anexo VI: Computational methods

25	1	0	-3.344511	2.969098	-5.919482
26	1	0	-2.043723	4.193889	-5.539551
27	15	0	1.219911	1.029976	-0.589185
28	15	0	-2.300917	0.076788	0.137082
29	29	0	-0.131960	-0.630078	0.480674
30	6	0	2.981231	0.523322	-0.904524
31	6	0	3.241709	-0.668789	-1.582462
32	6	0	4.035531	1.280224	-0.397753
33	6	0	4.554974	-1.118999	-1.787409
34	1	0	2.420548	-1.284181	-1.969905
35	6	0	5.368055	0.865272	-0.545956
36	1	0	3.845984	2.215340	0.141590
37	6	0	5.599682	-0.372948	-1.190133
38	6	0	1.423116	2.751351	0.060031
39	6	0	1.044762	3.032848	1.368489
40	6	0	1.943432	3.746380	-0.768121
41	6	0	1.209164	4.325687	1.896538
42	1	0	0.622146	2.249991	2.016845
43	6	0	2.158678	5.043079	-0.281784
44	1	0	2.202757	3.521411	-1.808670
45	6	0	1.846025	5.282349	1.076895
46	6	0	-3.337313	-0.117976	1.669946
47	6	0	-4.721613	-0.273043	1.578827
48	6	0	-2.708253	-0.151927	2.911842
49	6	0	-5.497348	-0.540141	2.715007
50	1	0	-5.226460	-0.208399	0.607292
51	6	0	-3.437591	-0.394502	4.088740
52	1	0	-1.619517	-0.001427	3.006216
53	6	0	-4.816084	-0.665298	3.949217
54	6	0	-3.407826	-0.794891	-1.067456
55	6	0	-3.657399	-2.135870	-0.756551
56	6	0	-4.008409	-0.196817	-2.167734

Anexo VI: Computational methods

57	6	0	-4.569619	-2.894222	-1.499313
58	1	0	-3.163103	-2.613657	0.098815
59	6	0	-4.929620	-0.915975	-2.955041
60	1	0	-3.783554	0.843842	-2.434669
61	6	0	-5.244772	-2.231970	-2.553376
62	7	0	1.183411	-2.159674	0.841652
63	6	0	1.604539	-3.111588	0.023929
64	6	0	1.996679	-1.976951	2.047684
65	1	0	2.603075	-3.532079	0.153963
66	6	0	0.866602	-3.644636	-1.129706
67	6	0	1.466482	-4.702738	-1.863340
68	6	0	-0.408050	-3.180405	-1.541561
69	6	0	0.816374	-5.272623	-2.969089
70	1	0	2.441925	-5.076398	-1.557372
71	6	0	-1.054672	-3.744901	-2.650827
72	1	0	-0.892544	-2.379297	-0.987271
73	6	0	-0.446736	-4.794019	-3.371374
74	1	0	1.290769	-6.083127	-3.515715
75	1	0	-2.032426	-3.369006	-2.953421
76	1	0	-0.949456	-5.230164	-4.231030
77	6	0	-4.804814	-4.363850	-1.117243
78	6	0	-6.069811	-4.437211	-0.239447
79	1	0	-6.973797	-4.187248	-0.814069
80	1	0	-6.212778	-5.444347	0.164828
81	1	0	-6.017099	-3.739442	0.611327
82	6	0	-4.955308	-5.243074	-2.369705
83	1	0	-5.821105	-4.950408	-2.979752
84	1	0	-4.075210	-5.166659	-3.016625
85	1	0	-5.084204	-6.296874	-2.105508
86	6	0	-3.618570	-4.933012	-0.307007
87	1	0	-2.678663	-4.875291	-0.869567
88	1	0	-3.473760	-4.413075	0.645759

Anexo VI: Computational methods

89	1	0	-3.779401	-5.990799	-0.069955
90	6	0	-5.556973	-0.232160	-4.178847
91	6	0	-4.625382	0.866620	-4.731031
92	1	0	-4.420663	1.651757	-3.989347
93	1	0	-3.658959	0.450983	-5.040887
94	1	0	-5.072384	1.350074	-5.604891
95	6	0	-5.794910	-1.224759	-5.329632
96	1	0	-6.573396	-1.960500	-5.095089
97	1	0	-6.100442	-0.711198	-6.245841
98	1	0	-4.886887	-1.795989	-5.552791
99	6	0	-6.880809	0.423668	-3.737437
100	1	0	-7.376930	0.917109	-4.579368
101	1	0	-7.584546	-0.318990	-3.333353
102	1	0	-6.714588	1.178670	-2.962637
103	6	0	2.735355	6.102148	-1.231001
104	6	0	0.697376	4.612414	3.315375
105	6	0	1.856634	4.379862	4.303530
106	1	0	2.205447	3.341901	4.271271
107	1	0	2.714939	5.029047	4.077171
108	1	0	1.547846	4.590897	5.332353
109	6	0	-0.463397	3.657649	3.676143
110	1	0	-1.296901	3.759709	2.972422
111	1	0	-0.148955	2.605123	3.673544
112	1	0	-0.849523	3.874292	4.677455
113	6	0	0.153201	6.045464	3.439117
114	1	0	-0.596496	6.252497	2.667463
115	1	0	-0.313533	6.213872	4.413757
116	1	0	0.940965	6.800005	3.319179
117	6	0	4.265779	6.119955	-1.055738
118	1	0	4.737045	6.831351	-1.740999
119	1	0	4.548142	6.410732	-0.032571
120	1	0	4.706661	5.131541	-1.247278

Anexo VI: Computational methods

121	6	0	2.142307	7.493562	-0.947582
122	1	0	2.456512	7.883477	0.030484
123	1	0	2.447322	8.224144	-1.701614
124	1	0	1.043109	7.457808	-0.925696
125	6	0	2.404373	5.760666	-2.702186
126	1	0	2.916954	4.853110	-3.040591
127	1	0	1.328608	5.603771	-2.847637
128	1	0	2.716657	6.567075	-3.373504
129	6	0	6.494289	1.759374	-0.006170
130	6	0	6.944516	1.202559	1.358998
131	1	0	6.129666	1.211823	2.086302
132	1	0	7.304754	0.164680	1.266767
133	1	0	7.770898	1.789732	1.772512
134	6	0	6.015348	3.216442	0.201160
135	1	0	5.650196	3.660800	-0.734798
136	1	0	5.211479	3.286646	0.941331
137	1	0	6.839082	3.844217	0.557065
138	6	0	7.673473	1.809081	-0.991055
139	1	0	8.452826	2.498369	-0.655989
140	1	0	8.144430	0.820984	-1.113354
141	1	0	7.348817	2.122024	-1.988242
142	6	0	4.782481	-2.380015	-2.637131
143	6	0	3.611334	-2.590684	-3.627243
144	1	0	2.651825	-2.734395	-3.118732
145	1	0	3.512587	-1.744797	-4.313608
146	1	0	3.781703	-3.484653	-4.238093
147	6	0	6.057818	-2.260582	-3.487711
148	1	0	6.061679	-1.342081	-4.081668
149	1	0	6.967408	-2.238249	-2.870990
150	1	0	6.163431	-3.109078	-4.170808
151	6	0	4.867023	-3.592229	-1.696067
152	1	0	5.745491	-3.533699	-1.028522

153	1	0	3.988420	-3.683977	-1.047594
154	1	0	4.975885	-4.528759	-2.254089
155	8	0	6.918074	-0.808346	-1.325693
156	8	0	-6.203023	-2.951585	-3.280069
157	8	0	-5.561385	-0.996598	5.088950
158	8	0	2.117608	6.553054	1.605234
159	6	0	3.418132	6.650437	2.240849
160	1	0	4.210392	6.470013	1.498344
161	1	0	3.430418	7.687531	2.593105
162	1	0	3.479083	5.943105	3.082650
163	6	0	-5.593813	-2.417349	5.379279
164	1	0	-6.177939	-2.453424	6.305320
165	1	0	-6.103741	-2.951873	4.563509
166	1	0	-4.571898	-2.796765	5.536806
167	6	0	-2.690453	-0.378439	5.431595
168	6	0	-1.442826	0.529265	5.354999
169	1	0	-0.738250	0.211778	4.570320
170	1	0	-1.719291	1.568733	5.152430
171	1	0	-0.888514	0.515562	6.298887
172	6	0	-3.573834	0.172183	6.563854
173	1	0	-4.421965	-0.486211	6.788159
174	1	0	-3.004552	0.296656	7.489684
175	1	0	-3.998756	1.145705	6.297398
176	6	0	-2.234814	-1.817253	5.743760
177	1	0	-1.704011	-1.865705	6.700175
178	1	0	-3.088380	-2.507981	5.806995
179	1	0	-1.557328	-2.198160	4.972190
180	6	0	-7.014037	-0.714846	2.553231
181	6	0	-7.526886	-0.001880	1.279491
182	1	0	-7.312825	1.071726	1.312163
183	1	0	-7.078817	-0.408822	0.366567
184	1	0	-8.612188	-0.111751	1.183176

185	6	0	-7.779556	-0.109800	3.741226
186	1	0	-7.552101	-0.625581	4.684565
187	1	0	-7.512095	0.941396	3.892035
188	1	0	-8.861553	-0.164041	3.593255
189	6	0	-7.307732	-2.222385	2.422349
190	1	0	-8.372840	-2.407231	2.255423
191	1	0	-6.751376	-2.672433	1.584735
192	1	0	-7.020914	-2.766066	3.335279
193	6	0	-7.561741	-2.794249	-2.799327
194	1	0	-8.134494	-3.383139	-3.524532
195	1	0	-7.649802	-3.216088	-1.786671
196	1	0	-7.856105	-1.733979	-2.824107
197	6	0	7.368810	-1.751038	-0.314818
198	1	0	8.376012	-2.012651	-0.665635
199	1	0	7.402128	-1.254655	0.663610
200	1	0	6.732438	-2.650810	-0.299428
201	1	0	3.072244	-1.968537	1.809055
202	6	0	1.597172	-0.701866	2.769096
203	8	0	0.486709	-0.139064	2.611391
204	8	0	2.434712	-0.151766	3.710321
205	6	0	3.860403	-0.498679	3.847577
206	1	0	4.372921	-0.454018	2.879097
207	1	0	4.261340	0.265028	4.514824
208	1	0	3.978570	-1.485925	4.301359
209	6	0	2.196439	-4.548440	2.456538
210	6	0	1.797171	-3.246848	3.066798
211	1	0	1.400559	-5.240791	2.192362
212	1	0	2.378315	-3.000695	3.967231
213	6	0	3.516622	-4.879915	2.109977
214	6	0	3.824421	-6.081537	1.352662
215	6	0	4.648024	-4.012748	2.393343
216	6	0	5.086505	-6.329832	0.843973

217	1	0	3.018964	-6.790299	1.165277
218	6	0	5.911340	-4.255341	1.880614
219	1	0	4.511652	-3.164972	3.057698
220	6	0	6.141699	-5.391997	1.062045
221	1	0	5.298195	-7.219441	0.259492
222	1	0	6.746314	-3.596412	2.093480
223	7	0	7.417179	-5.582520	0.461863
224	8	0	8.308086	-4.632918	0.575863
225	8	0	7.650115	-6.668144	-0.207189
226	1	0	0.738127	-3.255411	3.347319

INT2a

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	0.161214	-0.259693	-3.585847
2	6	0	-0.387894	-0.684653	-2.379262
3	6	0	-1.512379	0.063154	-1.896835
4	6	0	-2.038615	1.118398	-2.668094
5	6	0	-1.472439	1.513925	-3.904802
6	6	0	-0.352515	0.816454	-4.323613
7	1	0	-2.914840	1.658480	-2.316256
8	1	0	-1.892029	2.324803	-4.489106
9	6	0	0.078160	-1.973038	-1.767432
10	6	0	1.037087	-2.132548	-0.718910
11	6	0	-0.439350	-3.158452	-2.295380
12	6	0	1.394768	-3.419316	-0.264396
13	6	0	-0.075381	-4.432957	-1.835566
14	6	0	0.843806	-4.601860	-0.812198
15	1	0	2.122252	-3.518087	0.539335

16	1	0	1.129057	-5.584264	-0.454613
17	8	0	1.256912	-0.834115	-4.276094
18	8	0	0.384871	0.985057	-5.515879
19	8	0	-0.733914	-5.430712	-2.575256
20	8	0	-1.357686	-3.279523	-3.361040
21	6	0	1.573764	0.130215	-5.352320
22	6	0	-1.679257	-4.717586	-3.461817
23	1	0	-2.710379	-4.891970	-3.107582
24	1	0	-1.519405	-5.045766	-4.490183
25	1	0	2.420514	0.752245	-5.035264
26	1	0	1.753807	-0.415152	-6.279166
27	15	0	-2.095261	-0.295875	-0.119653
28	15	0	1.868787	-0.634222	0.077975
29	29	0	0.877530	1.345769	0.327378
30	6	0	-3.574355	0.840327	0.056376
31	6	0	-3.353937	2.216361	-0.007382
32	6	0	-4.846331	0.340686	0.323131
33	6	0	-4.413039	3.123568	0.157721
34	1	0	-2.341905	2.615867	-0.185108
35	6	0	-5.932587	1.202825	0.542771
36	1	0	-5.022138	-0.738769	0.384671
37	6	0	-5.669001	2.589847	0.520856
38	6	0	-2.954259	-1.946684	-0.336710
39	6	0	-2.692271	-2.918167	0.623683
40	6	0	-3.797458	-2.208550	-1.412774
41	6	0	-3.305641	-4.180536	0.554369
42	1	0	-2.006103	-2.711408	1.452108
43	6	0	-4.451343	-3.445360	-1.522547
44	1	0	-3.962113	-1.446567	-2.181731
45	6	0	-4.238075	-4.383856	-0.486585
46	6	0	2.280455	-1.322610	1.749649
47	6	0	3.525762	-1.876009	2.046450

48	6	0	1.287204	-1.259077	2.723279
49	6	0	3.836395	-2.297710	3.346379
50	1	0	4.295971	-1.972103	1.272449
51	6	0	1.525518	-1.717733	4.030601
52	1	0	0.302954	-0.810151	2.511108
53	6	0	2.836970	-2.136214	4.334814
54	6	0	3.539196	-0.592849	-0.722684
55	6	0	4.515854	0.206184	-0.127137
56	6	0	3.830124	-1.345493	-1.855359
57	6	0	5.837401	0.197379	-0.595120
58	1	0	4.270478	0.839091	0.734935
59	6	0	5.136767	-1.387007	-2.372780
60	1	0	3.044759	-1.923656	-2.360098
61	6	0	6.132172	-0.668660	-1.674164
62	7	0	0.231646	3.122607	0.493189
63	6	0	0.514631	4.308368	-0.323232
64	6	0	-0.323255	3.636681	1.737259
65	1	0	-0.427220	4.751055	-0.726374
66	6	0	1.431214	4.034883	-1.505958
67	6	0	1.044428	4.386795	-2.814436
68	6	0	2.697514	3.432804	-1.320721
69	6	0	1.891906	4.145708	-3.913649
70	1	0	0.072675	4.850226	-2.973443
71	6	0	3.549428	3.188526	-2.411693
72	1	0	3.008044	3.148848	-0.317477
73	6	0	3.149365	3.544932	-3.716663
74	1	0	1.570644	4.419845	-4.915902
75	1	0	4.518391	2.717243	-2.247813
76	1	0	3.811158	3.365461	-4.562127
77	6	0	6.869552	1.090409	0.108062
78	6	0	7.551108	0.254040	1.209973
79	1	0	8.070670	-0.618362	0.786531

80	1	0	8.294332	0.846263	1.752471
81	1	0	6.823896	-0.122260	1.947454
82	6	0	7.909396	1.642778	-0.880709
83	1	0	8.528254	0.850073	-1.319754
84	1	0	7.423678	2.154834	-1.718819
85	1	0	8.584125	2.355400	-0.398182
86	6	0	6.187645	2.312492	0.765964
87	1	0	5.651760	2.916897	0.024790
88	1	0	5.471094	2.023888	1.543008
89	1	0	6.927830	2.965054	1.240805
90	6	0	5.408047	-2.221655	-3.632797
91	6	0	4.121720	-2.398688	-4.470716
92	1	0	3.340757	-2.946846	-3.929229
93	1	0	3.695911	-1.431806	-4.756428
94	1	0	4.324748	-2.957809	-5.389327
95	6	0	6.445637	-1.540359	-4.541236
96	1	0	7.432419	-1.476222	-4.062989
97	1	0	6.573182	-2.081892	-5.482377
98	1	0	6.149615	-0.513425	-4.779120
99	6	0	5.897284	-3.616441	-3.194182
100	1	0	6.109422	-4.251094	-4.060392
101	1	0	6.820887	-3.551624	-2.600580
102	1	0	5.146396	-4.128861	-2.584466
103	6	0	-5.354467	-3.694166	-2.737781
104	6	0	-2.929117	-5.240943	1.598149
105	6	0	-3.959177	-5.183787	2.743674
106	1	0	-3.967266	-4.199987	3.223399
107	1	0	-4.977086	-5.383499	2.377765
108	1	0	-3.735549	-5.927773	3.514352
109	6	0	-1.524623	-4.970142	2.186543
110	1	0	-0.766530	-4.918315	1.396608
111	1	0	-1.476581	-4.028597	2.758724

112	1	0	-1.227986	-5.769774	2.872702
113	6	0	-2.885575	-6.645250	0.971471
114	1	0	-2.219726	-6.666787	0.101048
115	1	0	-2.531881	-7.393984	1.684848
116	1	0	-3.872703	-6.968645	0.616142
117	6	0	-6.800670	-3.331374	-2.348763
118	1	0	-7.485529	-3.468698	-3.190736
119	1	0	-7.161806	-3.959861	-1.520990
120	1	0	-6.877305	-2.285422	-2.022638
121	6	0	-5.268582	-5.157753	-3.207268
122	1	0	-5.706334	-5.850109	-2.475562
123	1	0	-5.790692	-5.310128	-4.155285
124	1	0	-4.221751	-5.467097	-3.335689
125	6	0	-4.926989	-2.811844	-3.933558
126	1	0	-5.086386	-1.745414	-3.737251
127	1	0	-3.864551	-2.941923	-4.172789
128	1	0	-5.501638	-3.058318	-4.831651
129	6	0	-7.320471	0.603189	0.804313
130	6	0	-7.548321	0.555312	2.328762
131	1	0	-6.792028	-0.061473	2.824394
132	1	0	-7.495348	1.561064	2.771590
133	1	0	-8.531217	0.141535	2.571385
134	6	0	-7.425581	-0.838805	0.252786
135	1	0	-7.227149	-0.873734	-0.826393
136	1	0	-6.718288	-1.518394	0.741439
137	1	0	-8.429377	-1.243683	0.413983
138	6	0	-8.420155	1.429016	0.114963
139	1	0	-9.404285	0.968862	0.232304
140	1	0	-8.480937	2.447746	0.524102
141	1	0	-8.221058	1.536292	-0.956250
142	6	0	-4.140157	4.617959	-0.061576
143	6	0	-3.026325	4.819237	-1.112770

144	1	0	-2.045043	4.437329	-0.776032
145	1	0	-3.269987	4.313926	-2.052019
146	1	0	-2.884777	5.881173	-1.339138
147	6	0	-5.381081	5.358623	-0.590913
148	1	0	-5.805170	4.842384	-1.459413
149	1	0	-6.182861	5.416186	0.153969
150	1	0	-5.139840	6.381593	-0.892335
151	6	0	-3.682064	5.220217	1.282481
152	1	0	-4.440503	5.065214	2.063211
153	1	0	-2.740539	4.748324	1.617963
154	1	0	-3.506532	6.296295	1.195836
155	8	0	-6.722764	3.471815	0.816951
156	8	0	7.460640	-0.760218	-2.116710
157	8	0	3.161606	-2.445533	5.665047
158	8	0	-4.928801	-5.605768	-0.543844
159	6	0	-6.191288	-5.593834	0.168356
160	1	0	-6.865745	-4.846433	-0.276807
161	1	0	-6.562326	-6.611471	0.008452
162	1	0	-6.016543	-5.396524	1.237433
163	6	0	3.601225	-1.284764	6.418609
164	1	0	3.780323	-1.702215	7.414235
165	1	0	4.526917	-0.887059	5.975897
166	1	0	2.802474	-0.525445	6.439017
167	6	0	0.361059	-1.676970	5.030151
168	6	0	-0.985676	-1.883217	4.296137
169	1	0	-1.184926	-1.071926	3.581880
170	1	0	-1.008741	-2.836379	3.746573
171	1	0	-1.818557	-1.889699	5.005583
172	6	0	0.471752	-2.789529	6.086013
173	1	0	1.347133	-2.658469	6.733686
174	1	0	-0.410804	-2.816073	6.730833
175	1	0	0.577665	-3.772451	5.615625

176	6	0	0.360127	-0.285324	5.688660
177	1	0	-0.451305	-0.182531	6.413206
178	1	0	1.306500	-0.084298	6.209009
179	1	0	0.225678	0.507826	4.931915
180	6	0	5.237317	-2.856316	3.626300
181	6	0	5.847328	-3.491362	2.353523
182	1	0	5.227016	-4.316828	1.989205
183	1	0	5.954751	-2.766264	1.538989
184	1	0	6.842711	-3.896743	2.560485
185	6	0	5.208907	-3.954313	4.702198
186	1	0	4.916248	-3.558427	5.684384
187	1	0	4.478352	-4.731850	4.454720
188	1	0	6.185049	-4.431819	4.819035
189	6	0	6.132637	-1.681027	4.069589
190	1	0	7.127724	-2.026956	4.362929
191	1	0	6.259006	-0.944586	3.260271
192	1	0	5.696728	-1.154970	4.932491
193	6	0	8.225929	-1.801988	-1.460256
194	1	0	9.212008	-1.697124	-1.925288
195	1	0	8.272444	-1.611519	-0.376996
196	1	0	7.783673	-2.785914	-1.680627
197	6	0	-6.748157	3.886239	2.206119
198	1	0	-7.587681	4.588469	2.228835
199	1	0	-6.941316	3.012141	2.847081
200	1	0	-5.802587	4.381946	2.472604
201	1	0	-1.396372	3.958293	1.632155
202	6	0	-0.296366	2.582854	2.843719
203	8	0	0.238864	1.466730	2.723892
204	8	0	-0.915438	2.842706	4.059006
205	6	0	-1.627579	4.090846	4.357312
206	1	0	-2.344351	4.344268	3.565631
207	1	0	-2.159372	3.889644	5.289244

208	1	0	-0.922152	4.914722	4.503629
209	6	0	1.112792	5.377127	0.702413
210	6	0	0.500309	4.948010	2.073932
211	1	0	2.196197	5.215262	0.736463
212	1	0	-0.126361	5.738145	2.500894
213	6	0	0.858022	6.821226	0.305597
214	6	0	1.927124	7.663986	-0.070246
215	6	0	-0.453340	7.354562	0.267175
216	6	0	1.701899	8.996126	-0.466120
217	1	0	2.942225	7.270839	-0.057376
218	6	0	-0.684901	8.683700	-0.127612
219	1	0	-1.299266	6.727096	0.546206
220	6	0	0.393166	9.513385	-0.495630
221	1	0	2.542542	9.625482	-0.750632
222	1	0	-1.700743	9.073270	-0.150829
223	1	0	1.299766	4.725652	2.791092
224	1	0	0.215365	10.542193	-0.800696

INT3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.156524	-0.396746	-3.571667
2	6	0	-0.404160	-0.860701	-2.384787
3	6	0	-1.514550	-0.110793	-1.873405
4	6	0	-2.018200	0.985246	-2.601806
5	6	0	-1.440378	1.421035	-3.819564
6	6	0	-0.332826	0.719787	-4.264568
7	1	0	-2.887148	1.525146	-2.232029
8	1	0	-1.844107	2.261693	-4.372052

9	6	0	0.030563	-2.185359	-1.829713
10	6	0	0.984260	-2.415306	-0.789358
11	6	0	-0.515521	-3.332890	-2.409838
12	6	0	1.309439	-3.729412	-0.392317
13	6	0	-0.183990	-4.635318	-2.006985
14	6	0	0.729571	-4.872264	-0.992146
15	1	0	2.033438	-3.882266	0.406021
16	1	0	0.989831	-5.876298	-0.678508
17	8	0	1.240395	-0.965793	-4.283674
18	8	0	0.410741	0.923720	-5.446858
19	8	0	-0.866958	-5.582087	-2.789407
20	8	0	-1.435677	-3.383094	-3.478962
21	6	0	1.574478	0.027404	-5.328055
22	6	0	-1.790439	-4.807410	-3.647016
23	1	0	-2.827223	-4.973268	-3.305988
24	1	0	-1.632176	-5.091993	-4.688481
25	1	0	2.443808	0.610976	-4.999513
26	1	0	1.727939	-0.488827	-6.276182
27	15	0	-2.110918	-0.532489	-0.114320
28	15	0	1.852888	-0.976928	0.072606
29	29	0	0.901167	1.010121	0.410933
30	6	0	-3.567480	0.625478	0.107089
31	6	0	-3.322237	1.998655	0.092393
32	6	0	-4.848115	0.140272	0.358411
33	6	0	-4.363904	2.918843	0.291887
34	1	0	-2.303978	2.384175	-0.074328
35	6	0	-5.918603	1.013814	0.608569
36	1	0	-5.043615	-0.937473	0.382590
37	6	0	-5.630073	2.395849	0.635511
38	6	0	-3.002511	-2.153616	-0.400160
39	6	0	-2.760007	-3.171925	0.515913
40	6	0	-3.853141	-2.349541	-1.484478

Anexo VI: Computational methods

41	6	0	-3.400698	-4.416427	0.392534
42	1	0	-2.068332	-3.016808	1.350923
43	6	0	-4.533884	-3.565782	-1.646953
44	1	0	-4.002910	-1.551045	-2.218680
45	6	0	-4.338987	-4.553716	-0.654128
46	6	0	2.248015	-1.745882	1.711828
47	6	0	3.479783	-2.341870	1.981495
48	6	0	1.256548	-1.703410	2.688575
49	6	0	3.780377	-2.830047	3.260338
50	1	0	4.247406	-2.421323	1.202944
51	6	0	1.484078	-2.226758	3.973156
52	1	0	0.282777	-1.223444	2.497873
53	6	0	2.785269	-2.690242	4.256411
54	6	0	3.522745	-0.934325	-0.726623
55	6	0	4.517633	-0.187250	-0.094654
56	6	0	3.796718	-1.640284	-1.893066
57	6	0	5.838639	-0.204780	-0.563439
58	1	0	4.287034	0.408835	0.797006
59	6	0	5.102363	-1.688131	-2.412604
60	1	0	2.998541	-2.176496	-2.423619
61	6	0	6.113873	-1.026006	-1.682263
62	7	0	0.283886	2.792754	0.652853
63	6	0	0.582992	4.001587	-0.111160
64	6	0	-0.294251	3.258020	1.904472
65	1	0	-0.350028	4.481743	-0.493414
66	6	0	1.504109	3.772961	-1.298855
67	6	0	1.124234	4.179553	-2.593307
68	6	0	2.765327	3.155288	-1.131455
69	6	0	1.975090	3.977493	-3.697573
70	1	0	0.154580	4.651737	-2.739320
71	6	0	3.620522	2.950573	-2.227940
72	1	0	3.069520	2.826835	-0.139782

Anexo VI: Computational methods

73	6	0	3.228045	3.361955	-3.518875
74	1	0	1.659841	4.292747	-4.689319
75	1	0	4.585469	2.466577	-2.079789
76	1	0	3.892208	3.212239	-4.367905
77	6	0	6.891659	0.629166	0.180291
78	6	0	7.554670	-0.274784	1.239028
79	1	0	8.053664	-1.137560	0.773001
80	1	0	8.312519	0.272956	1.807616
81	1	0	6.820164	-0.669526	1.959425
82	6	0	7.942786	1.205140	-0.782537
83	1	0	8.543530	0.420665	-1.260277
84	1	0	7.469049	1.767796	-1.594481
85	1	0	8.634462	1.877759	-0.267472
86	6	0	6.238579	1.833260	0.898561
87	1	0	5.717521	2.485682	0.188792
88	1	0	5.516658	1.522999	1.662066
89	1	0	6.994914	2.443400	1.403781
90	6	0	5.354889	-2.470891	-3.709491
91	6	0	4.065322	-2.579251	-4.554063
92	1	0	3.270427	-3.131108	-4.037174
93	1	0	3.664398	-1.590694	-4.797989
94	1	0	4.255589	-3.103081	-5.496088
95	6	0	6.408754	-1.773869	-4.586535
96	1	0	7.396865	-1.755294	-4.107115
97	1	0	6.523836	-2.275152	-5.551445
98	1	0	6.137768	-0.730483	-4.777817
99	6	0	5.810467	-3.895214	-3.334624
100	1	0	6.007785	-4.494980	-4.228911
101	1	0	6.735408	-3.879799	-2.739716
102	1	0	5.047536	-4.417062	-2.748327
103	6	0	-5.444990	-3.740528	-2.869253
104	6	0	-3.046060	-5.529914	1.387719

105	6	0	-4.074288	-5.502414	2.535877
106	1	0	-4.062255	-4.541088	3.058993
107	1	0	-5.096282	-5.665181	2.163003
108	1	0	-3.865781	-6.284451	3.272494
109	6	0	-1.636145	-5.314995	1.986195
110	1	0	-0.877115	-5.243976	1.198778
111	1	0	-1.568549	-4.401574	2.600323
112	1	0	-1.356460	-6.150850	2.635476
113	6	0	-3.031831	-6.905328	0.698893
114	1	0	-2.367145	-6.902051	-0.172648
115	1	0	-2.693471	-7.692443	1.377652
116	1	0	-4.025651	-7.192421	0.331072
117	6	0	-6.882249	-3.365956	-2.459207
118	1	0	-7.571425	-3.447930	-3.304992
119	1	0	-7.255845	-4.025818	-1.661920
120	1	0	-6.936222	-2.335296	-2.082872
121	6	0	-5.390130	-5.182637	-3.404850
122	1	0	-5.838551	-5.898968	-2.703240
123	1	0	-5.919498	-5.281603	-4.356032
124	1	0	-4.350336	-5.506482	-3.553005
125	6	0	-5.002608	-2.813768	-4.025360
126	1	0	-5.139370	-1.754287	-3.780535
127	1	0	-3.944179	-2.955193	-4.275131
128	1	0	-5.585392	-3.007249	-4.931330
129	6	0	-7.317582	0.430022	0.847431
130	6	0	-7.549048	0.333064	2.368908
131	1	0	-6.804383	-0.313064	2.844277
132	1	0	-7.481815	1.321617	2.847003
133	1	0	-8.539203	-0.073080	2.595266
134	6	0	-7.446898	-0.989951	0.246422
135	1	0	-7.246239	-0.992501	-0.833220
136	1	0	-6.754242	-1.699103	0.713485

137	1	0	-8.458650	-1.381480	0.391109
138	6	0	-8.400755	1.298599	0.185481
139	1	0	-9.393351	0.852473	0.285956
140	1	0	-8.444837	2.303787	0.628709
141	1	0	-8.198573	1.438571	-0.881423
142	6	0	-4.064091	4.415055	0.127911
143	6	0	-2.940850	4.635770	-0.910240
144	1	0	-1.968854	4.225016	-0.584047
145	1	0	-3.189850	4.166568	-1.867444
146	1	0	-2.786003	5.702278	-1.102149
147	6	0	-5.288179	5.196366	-0.379860
148	1	0	-5.715422	4.721997	-1.270661
149	1	0	-6.095107	5.238283	0.360994
150	1	0	-5.029931	6.226763	-0.639627
151	6	0	-3.602484	4.959907	1.495583
152	1	0	-4.373361	4.795884	2.263175
153	1	0	-2.677817	4.453204	1.823781
154	1	0	-3.405721	6.034465	1.449054
155	8	0	-6.667696	3.286692	0.958413
156	8	0	7.439525	-1.125539	-2.130117
157	8	0	3.101617	-3.069486	5.570073
158	8	0	-5.054483	-5.757228	-0.764350
159	6	0	-6.316063	-5.752407	-0.050343
160	1	0	-6.976153	-4.972876	-0.460541
161	1	0	-6.707000	-6.754498	-0.255357
162	1	0	-6.136881	-5.606990	1.026264
163	6	0	3.571076	-1.957648	6.377465
164	1	0	3.740215	-2.427158	7.351593
165	1	0	4.506482	-1.562847	5.952961
166	1	0	2.791798	-1.180481	6.436191
167	6	0	0.321193	-2.205494	4.975260
168	6	0	-1.030545	-2.343075	4.234562

169	1	0	-1.210432	-1.494735	3.559566
170	1	0	-1.077755	-3.268792	3.641104
171	1	0	-1.862924	-2.362763	4.944517
172	6	0	0.405156	-3.369642	5.976288
173	1	0	1.283211	-3.291020	6.628925
174	1	0	-0.477855	-3.406306	6.620129
175	1	0	0.487547	-4.331312	5.459426
176	6	0	0.354711	-0.847367	5.699889
177	1	0	-0.452491	-0.761280	6.431556
178	1	0	1.306480	-0.694685	6.226960
179	1	0	0.237235	-0.016206	4.983063
180	6	0	5.167268	-3.435392	3.512417
181	6	0	5.761411	-4.025153	2.210766
182	1	0	5.121463	-4.817800	1.809321
183	1	0	5.886931	-3.266104	1.430570
184	1	0	6.746621	-4.464080	2.397692
185	6	0	5.111620	-4.581240	4.535901
186	1	0	4.829504	-4.224925	5.536135
187	1	0	4.362111	-5.328302	4.253555
188	1	0	6.075658	-5.087933	4.628964
189	6	0	6.091074	-2.304345	4.008967
190	1	0	7.077341	-2.688275	4.284853
191	1	0	6.236137	-1.534449	3.234779
192	1	0	5.668731	-1.808736	4.896264
193	6	0	8.182429	-2.214770	-1.526849
194	1	0	9.169802	-2.109285	-1.989296
195	1	0	8.235258	-2.077889	-0.435854
196	1	0	7.718188	-3.176951	-1.793265
197	6	0	-6.695975	3.651162	2.361363
198	1	0	-7.525309	4.364987	2.403619
199	1	0	-6.907171	2.758194	2.969890
200	1	0	-5.745389	4.122961	2.651226

201	1	0	-1.362877	3.588858	1.792081
202	6	0	-0.287138	2.159461	2.968369
203	8	0	0.249273	1.049436	2.809299
204	8	0	-0.922090	2.373349	4.182626
205	6	0	-1.647665	3.604817	4.517901
206	1	0	-2.350581	3.887007	3.723391
207	1	0	-2.196683	3.362163	5.429429
208	1	0	-0.949885	4.425033	4.714155
209	6	0	1.193855	5.015063	0.976715
210	6	0	0.528009	4.554144	2.310096
211	1	0	2.268663	4.810838	1.027173
212	1	0	-0.110496	5.333554	2.739642
213	6	0	0.995489	6.471090	0.622513
214	6	0	2.098837	7.285258	0.272910
215	6	0	-0.301117	7.046823	0.579133
216	6	0	1.932152	8.627328	-0.094746
217	1	0	3.098009	6.856932	0.287352
218	6	0	-0.492628	8.383533	0.213364
219	1	0	-1.168021	6.440456	0.833684
220	6	0	0.631961	9.163454	-0.117220
221	1	0	2.775332	9.255735	-0.359157
222	1	0	-1.479658	8.831182	0.178139
223	7	0	0.440793	10.570140	-0.494466
224	8	0	-0.752754	11.040472	-0.506032
225	8	0	1.474778	11.266289	-0.794410
226	1	0	1.299540	4.307204	3.048851

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	7	0	1.384504	-0.724649	1.360617
2	6	0	-0.030192	-0.441963	0.991524
3	6	0	2.319547	0.262367	0.816179
4	1	0	-0.561587	-0.036569	1.865184
5	6	0	-0.793850	-1.671772	0.513010
6	6	0	-2.065706	-1.961707	1.048963
7	6	0	-0.257805	-2.528601	-0.477664
8	6	0	-2.798859	-3.078173	0.604367
9	1	0	-2.483770	-1.311568	1.815433
10	6	0	-0.987756	-3.646904	-0.918429
11	1	0	0.725819	-2.323877	-0.895016
12	6	0	-2.260669	-3.926129	-0.381545
13	1	0	-3.779102	-3.286835	1.027079
14	1	0	-0.564422	-4.300088	-1.678359
15	1	0	-2.821845	-4.792486	-0.724552
16	1	0	3.014881	0.623731	1.585603
17	6	0	3.153604	-0.286946	-0.364785
18	8	0	2.849638	-1.302013	-1.005223
19	8	0	4.294758	0.407865	-0.743832
20	6	0	4.830792	1.543195	0.020151
21	1	0	5.202357	1.213338	0.997508
22	1	0	5.662282	1.911969	-0.582947
23	1	0	4.087072	2.337250	0.145716
24	6	0	0.084943	0.700087	-0.082275
25	6	0	1.388661	1.425954	0.344091
26	1	0	0.259867	0.221470	-1.053821
27	1	0	1.196472	2.097023	1.189064
28	6	0	-1.135507	1.598200	-0.192267
29	6	0	-1.870970	1.657087	-1.395585
30	6	0	-1.571351	2.386214	0.899235
31	6	0	-3.005764	2.481692	-1.512882

32	1	0	-1.556031	1.050025	-2.242237
33	6	0	-2.704706	3.210461	0.787534
34	1	0	-1.028535	2.357476	1.842532
35	6	0	-3.426848	3.263531	-0.421193
36	1	0	-3.558502	2.511454	-2.449072
37	1	0	-3.025145	3.808940	1.637553
38	1	0	1.811558	2.020700	-0.472665
39	1	0	1.669934	-1.697023	1.299092
40	1	0	-4.303385	3.901235	-0.508542

exo-64a

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	7	0	2.462154	-0.004192	-1.314356
2	6	0	1.098474	0.511393	-1.017590
3	6	0	2.690013	-1.347250	-0.774633
4	1	0	0.479515	0.454861	-1.925546
5	6	0	1.082259	1.955850	-0.530851
6	6	0	0.222887	2.894102	-1.138703
7	6	0	1.909292	2.375647	0.538180
8	6	0	0.175120	4.226416	-0.686224
9	1	0	-0.408712	2.583525	-1.969354
10	6	0	1.865150	3.707468	0.986898
11	1	0	2.588509	1.667608	1.008557
12	6	0	0.997199	4.637179	0.379532
13	1	0	-0.493869	4.938072	-1.164371
14	1	0	2.507245	4.020413	1.807109
15	1	0	0.965836	5.666402	0.729427
16	1	0	3.122297	-2.016066	-1.529758
17	6	0	3.616172	-1.343997	0.464835

18	8	0	3.836212	-0.333881	1.146292
19	8	0	4.204888	-2.538070	0.851010
20	6	0	4.128974	-3.767178	0.047302
21	1	0	4.674970	-3.648729	-0.895861
22	1	0	4.616803	-4.526242	0.660863
23	1	0	3.092399	-4.062903	-0.147808
24	6	0	0.534120	-0.523452	0.025257
25	6	0	1.256758	-1.834162	-0.385266
26	1	0	0.899144	-0.223822	1.014782
27	1	0	0.779108	-2.283218	-1.263639
28	6	0	-0.978035	-0.613260	0.068551
29	6	0	-1.677714	-0.251916	1.242273
30	6	0	-1.724091	-1.038865	-1.058356
31	6	0	-3.077161	-0.315951	1.306457
32	1	0	-1.119523	0.086914	2.111256
33	6	0	-3.122117	-1.109778	-1.017664
34	1	0	-1.212542	-1.316078	-1.976612
35	6	0	-3.782205	-0.748000	0.170626
36	1	0	-3.620657	-0.040438	2.203271
37	1	0	-3.702896	-1.434422	-1.873848
38	7	0	-5.253183	-0.823124	0.223483
39	8	0	-5.877016	-1.215684	-0.823964
40	8	0	-5.837899	-0.493295	1.313543
41	1	0	1.251988	-2.575886	0.420485
42	1	0	3.217546	0.663182	-1.191622

ET1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-0.737111	-2.994192	-3.089424
2	6	0	-0.948785	-2.310036	-1.889981
3	6	0	-1.682191	-1.083015	-2.007588
4	6	0	-2.113437	-0.626066	-3.271001
5	6	0	-1.867551	-1.341296	-4.467310
6	6	0	-1.181770	-2.538159	-4.336444
7	1	0	-2.681780	0.299164	-3.341075
8	1	0	-2.214785	-0.979543	-5.427891
9	6	0	-0.543010	-3.014190	-0.622434
10	6	0	0.543695	-2.694116	0.261714
11	6	0	-1.226496	-4.197367	-0.324651
12	6	0	0.859313	-3.553738	1.336683
13	6	0	-0.903752	-5.035440	0.751712
14	6	0	0.145201	-4.744420	1.606320
15	1	0	1.685202	-3.301879	1.999014
16	1	0	0.410116	-5.391973	2.433343
17	8	0	-0.053243	-4.223235	-3.248718
18	8	0	-0.816912	-3.452215	-5.349131
19	8	0	-1.739840	-6.168428	0.763365
20	8	0	-2.296465	-4.760607	-1.059180
21	6	0	-0.348260	-4.653524	-4.628902
22	6	0	-2.769310	-5.910041	-0.260128
23	1	0	-3.718534	-5.641436	0.239541
24	1	0	-2.858279	-6.782685	-0.908085
25	1	0	0.567505	-5.018926	-5.095279
26	1	0	-1.153827	-5.397583	-4.608810
27	15	0	-2.016142	-0.049600	-0.456810
28	15	0	1.478457	-1.049223	0.152738
29	29	0	0.022379	0.758477	0.414405
30	6	0	-3.181052	1.269915	-1.053577
31	6	0	-2.649668	2.294895	-1.839919

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32	6	0	-4.521387	1.294217	-0.679690
33	6	0	-3.448685	3.363257	-2.274189
34	1	0	-1.589058	2.295900	-2.125403
35	6	0	-5.359418	2.358023	-1.054709
36	1	0	-4.948055	0.492614	-0.065449
37	6	0	-4.776567	3.411996	-1.791257
38	6	0	-3.110013	-1.155380	0.545079
39	6	0	-2.906555	-1.197262	1.919779
40	6	0	-4.089636	-1.944411	-0.059534
41	6	0	-3.708899	-2.009845	2.740573
42	1	0	-2.114781	-0.593220	2.398507
43	6	0	-4.933909	-2.754205	0.712457
44	1	0	-4.210215	-1.933846	-1.147617
45	6	0	-4.761758	-2.712152	2.117778
46	6	0	2.697241	-1.208049	1.551551
47	6	0	3.948542	-1.793660	1.357500
48	6	0	2.349632	-0.688586	2.795970
49	6	0	4.910676	-1.798694	2.377125
50	1	0	4.210266	-2.243344	0.392173
51	6	0	3.265107	-0.688041	3.862182
52	1	0	1.351130	-0.253472	2.971739
53	6	0	4.564802	-1.169780	3.596285
54	6	0	2.661491	-1.147109	-1.273150
55	6	0	3.610515	-0.120673	-1.321686
56	6	0	2.676212	-2.167586	-2.212990
57	6	0	4.649293	-0.139999	-2.259949
58	1	0	3.568471	0.715147	-0.609595
59	6	0	3.705524	-2.243754	-3.175810
60	1	0	1.893777	-2.938320	-2.224520
61	6	0	4.714404	-1.260149	-3.126401
62	7	0	0.160417	2.745883	0.731771
63	6	0	0.617783	3.777026	-0.014109

64	6	0	0.050704	3.150027	2.107667
65	1	0	0.330174	4.791701	0.275365
66	6	0	1.094296	3.668003	-1.401293
67	6	0	1.374238	4.866818	-2.112035
68	6	0	1.300010	2.435734	-2.074370
69	6	0	1.841823	4.833053	-3.435341
70	1	0	1.232426	5.822717	-1.612765
71	6	0	1.761010	2.402222	-3.400224
72	1	0	1.108843	1.499946	-1.551836
73	6	0	2.036260	3.600246	-4.091502
74	1	0	2.053731	5.764769	-3.955283
75	1	0	1.913182	1.441828	-3.892858
76	1	0	2.396033	3.572522	-5.117756
77	6	0	5.641163	1.034482	-2.278033
78	6	0	6.863042	0.652811	-1.418164
79	1	0	7.458644	-0.140910	-1.892063
80	1	0	7.525476	1.511876	-1.271721
81	1	0	6.563017	0.290668	-0.422135
82	6	0	6.069897	1.382100	-3.713710
83	1	0	6.592593	0.552550	-4.206274
84	1	0	5.200085	1.618112	-4.336387
85	1	0	6.737424	2.248419	-3.731029
86	6	0	5.006465	2.309184	-1.680035
87	1	0	4.101122	2.606704	-2.225456
88	1	0	4.730011	2.190171	-0.625934
89	1	0	5.698523	3.156448	-1.730223
90	6	0	3.564445	-3.332194	-4.251012
91	6	0	2.500216	-2.815560	-5.244025
92	1	0	1.536858	-2.630622	-4.756466
93	1	0	2.818555	-1.870303	-5.699400
94	1	0	2.329978	-3.525677	-6.057614
95	6	0	4.844321	-3.642130	-5.041271

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96	1	0	5.635445	-4.032020	-4.393539
97	1	0	4.657473	-4.388689	-5.819299
98	1	0	5.233365	-2.742210	-5.540095
99	6	0	3.100756	-4.654194	-3.600022
100	1	0	3.025046	-5.455696	-4.339421
101	1	0	3.805316	-4.982847	-2.829776
102	1	0	2.115569	-4.554082	-3.120463
103	6	0	-5.986414	-3.622072	0.008964
104	6	0	-3.384134	-2.072912	4.240601
105	6	0	-4.230780	-1.006129	4.963125
106	1	0	-3.984044	0.000816	4.609668
107	1	0	-5.306212	-1.165735	4.800665
108	1	0	-4.053179	-1.027135	6.042978
109	6	0	-1.889514	-1.769732	4.488186
110	1	0	-1.245677	-2.504578	3.993941
111	1	0	-1.593588	-0.774497	4.116643
112	1	0	-1.655210	-1.789377	5.556692
113	6	0	-3.659936	-3.471495	4.818632
114	1	0	-3.147308	-4.245931	4.237295
115	1	0	-3.318329	-3.549767	5.854589
116	1	0	-4.726430	-3.725337	4.803225
117	6	0	-7.335685	-2.877750	0.034773
118	1	0	-8.124214	-3.470053	-0.439881
119	1	0	-7.658410	-2.666358	1.065120
120	1	0	-7.275194	-1.921734	-0.494865
121	6	0	-6.119546	-4.994778	0.692309
122	1	0	-6.504771	-4.904380	1.718510
123	1	0	-6.797797	-5.654992	0.146100
124	1	0	-5.141735	-5.493432	0.773220
125	6	0	-5.601078	-3.881833	-1.465989
126	1	0	-5.645275	-2.969145	-2.070124
127	1	0	-4.583059	-4.281951	-1.555491

Anexo VI: Computational methods

128	1	0	-6.282870	-4.601221	-1.929949
129	6	0	-6.834104	2.329851	-0.629385
130	6	0	-6.970049	3.124912	0.684430
131	1	0	-6.362860	2.685516	1.481890
132	1	0	-6.641993	4.167584	0.555135
133	1	0	-8.008306	3.149289	1.028615
134	6	0	-7.313729	0.880293	-0.380634
135	1	0	-7.216823	0.273176	-1.287171
136	1	0	-6.747963	0.388488	0.418967
137	1	0	-8.368317	0.864633	-0.087136
138	6	0	-7.745813	2.919066	-1.718840
139	1	0	-8.802927	2.808022	-1.463499
140	1	0	-7.557400	3.989948	-1.877538
141	1	0	-7.577535	2.429999	-2.684076
142	6	0	-2.837349	4.406841	-3.221263
143	6	0	-1.706884	3.779034	-4.067744
144	1	0	-0.862467	3.440944	-3.451931
145	1	0	-2.066138	2.926779	-4.650842
146	1	0	-1.296023	4.509467	-4.773461
147	6	0	-3.881941	4.953055	-4.209911
148	1	0	-4.390511	4.140394	-4.738737
149	1	0	-4.664154	5.535534	-3.707295
150	1	0	-3.421024	5.604755	-4.957726
151	6	0	-2.244981	5.544177	-2.368300
152	1	0	-3.010388	6.017428	-1.736369
153	1	0	-1.450328	5.176109	-1.708385
154	1	0	-1.808288	6.326452	-2.997625
155	8	0	-5.572845	4.521986	-2.110704
156	8	0	5.784732	-1.350137	-4.027315
157	8	0	5.540012	-1.085440	4.600800
158	8	0	-5.634810	-3.472371	2.911589
159	6	0	-6.771603	-2.724650	3.411783

160	1	0	-7.397969	-2.395939	2.568581
161	1	0	-7.289813	-3.467868	4.027034
162	1	0	-6.428592	-1.872728	4.019749
163	6	0	6.281841	0.161814	4.586846
164	1	0	6.948859	0.048374	5.447534
165	1	0	6.849395	0.244932	3.647486
166	1	0	5.595883	1.013469	4.720823
167	6	0	2.806553	-0.127041	5.216417
168	6	0	1.283176	-0.311623	5.397685
169	1	0	0.700343	0.209090	4.622697
170	1	0	1.001849	-1.368701	5.364401
171	1	0	0.950480	0.088531	6.360362
172	6	0	3.483531	-0.847834	6.394633
173	1	0	4.566024	-0.673931	6.422422
174	1	0	3.074887	-0.515102	7.352890
175	1	0	3.345319	-1.931952	6.326425
176	6	0	3.133602	1.378345	5.232338
177	1	0	2.771245	1.857675	6.145915
178	1	0	4.217500	1.556957	5.172422
179	1	0	2.673394	1.896247	4.376827
180	6	0	6.278344	-2.438660	2.102856
181	6	0	6.184989	-3.496715	0.977642
182	1	0	5.481904	-4.293991	1.241089
183	1	0	5.859953	-3.061485	0.026102
184	1	0	7.158363	-3.966152	0.803314
185	6	0	6.823272	-3.158535	3.347682
186	1	0	7.017722	-2.459898	4.173562
187	1	0	6.104898	-3.892786	3.726871
188	1	0	7.759503	-3.680585	3.133871
189	6	0	7.241291	-1.323595	1.649602
190	1	0	8.227214	-1.724603	1.399544
191	1	0	6.856383	-0.793416	0.763689

Anexo VI: Computational methods

192	1	0	7.382654	-0.572547	2.441740
193	6	0	6.948331	-2.027160	-3.483203
194	1	0	7.627058	-2.049894	-4.342720
195	1	0	7.372743	-1.435058	-2.657485
196	1	0	6.683412	-3.037878	-3.156518
197	6	0	-5.462464	5.608070	-1.155286
198	1	0	-6.121248	6.368827	-1.587050
199	1	0	-5.825590	5.274959	-0.171214
200	1	0	-4.420987	5.963433	-1.105115
201	1	0	-0.491768	4.101702	2.231161
202	6	0	-0.525090	2.066079	2.972116
203	8	0	-0.468351	0.844604	2.676756
204	8	0	-1.055606	2.374794	4.207324
205	6	0	-1.328372	3.758850	4.626834
206	1	0	-2.080142	4.219446	3.975142
207	1	0	-1.722968	3.664232	5.639937
208	1	0	-0.414044	4.360328	4.639654
209	6	0	2.342462	4.300491	1.594821
210	6	0	1.627132	3.529316	2.630344
211	1	0	3.100995	3.778474	1.016769
212	1	0	1.516373	4.068960	3.579721
213	6	0	2.366828	5.746457	1.553680
214	6	0	3.262537	6.434006	0.672640
215	6	0	1.476337	6.564441	2.320667
216	6	0	3.275767	7.831124	0.578554
217	1	0	3.952008	5.846176	0.068209
218	6	0	1.494565	7.965849	2.221362
219	1	0	0.778682	6.098691	3.014522
220	6	0	2.391325	8.617900	1.351965
221	1	0	3.978583	8.315633	-0.097702
222	1	0	0.806972	8.555315	2.826872
223	1	0	2.099737	2.557536	2.831104

224 1 0 2.405820 9.702851 1.280047

ET1b

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-2.145557	-3.398710	-2.325692
2	6	0	-1.968886	-2.432219	-1.332675
3	6	0	-2.263972	-1.086620	-1.731805
4	6	0	-2.668902	-0.803512	-3.053267
5	6	0	-2.820805	-1.809644	-4.037348
6	6	0	-2.562543	-3.108870	-3.631034
7	1	0	-2.908857	0.219969	-3.334267
8	1	0	-3.144888	-1.575947	-5.044475
9	6	0	-1.672405	-2.926167	0.058223
10	6	0	-0.448109	-2.807057	0.801453
11	6	0	-2.667113	-3.698701	0.666181
12	6	0	-0.311437	-3.450432	2.050714
13	6	0	-2.517065	-4.323433	1.912256
14	6	0	-1.341365	-4.223639	2.635124
15	1	0	0.620586	-3.356245	2.604105
16	1	0	-1.211308	-4.713086	3.592526
17	8	0	-1.941112	-4.791858	-2.190694
18	8	0	-2.654586	-4.296267	-4.388373
19	8	0	-3.670294	-5.061297	2.236557
20	8	0	-3.937434	-4.010768	0.129624
21	6	0	-2.539963	-5.388615	-3.400354
22	6	0	-4.666370	-4.714968	1.205778
23	1	0	-5.420020	-4.033705	1.641795

Anexo VI: Computational methods

24	1	0	-5.099106	-5.631313	0.803051
25	1	0	-1.873389	-6.158748	-3.789617
26	1	0	-3.542697	-5.760709	-3.158209
27	15	0	-2.084188	0.309218	-0.465726
28	15	0	0.962012	-1.666751	0.249527
29	29	0	0.175437	0.532297	0.197089
30	6	0	-2.820781	1.782661	-1.327513
31	6	0	-2.096221	2.359424	-2.373369
32	6	0	-4.024085	2.345875	-0.913220
33	6	0	-2.563838	3.505742	-3.032937
34	1	0	-1.137874	1.933941	-2.697093
35	6	0	-4.524272	3.513300	-1.514720
36	1	0	-4.600736	1.900728	-0.093403
37	6	0	-3.737378	4.109175	-2.523922
38	6	0	-3.369580	-0.127744	0.789890
39	6	0	-3.059372	0.032720	2.135360
40	6	0	-4.610726	-0.634196	0.397805
41	6	0	-4.003437	-0.268095	3.133349
42	1	0	-2.067199	0.402994	2.454635
43	6	0	-5.595631	-0.933229	1.348694
44	1	0	-4.829010	-0.799514	-0.662292
45	6	0	-5.285573	-0.669498	2.705392
46	6	0	2.225344	-1.943359	1.587991
47	6	0	3.200763	-2.931887	1.465340
48	6	0	2.188872	-1.127074	2.717562
49	6	0	4.211401	-3.076888	2.427198
50	1	0	3.207478	-3.608298	0.601789
51	6	0	3.155315	-1.249900	3.729039
52	1	0	1.402002	-0.362641	2.840208
53	6	0	4.204736	-2.171108	3.512359
54	6	0	1.843291	-2.485874	-1.163339
55	6	0	3.055310	-1.894837	-1.534951

Anexo VI: Computational methods

56	6	0	1.405742	-3.647864	-1.783541
57	6	0	3.901267	-2.506647	-2.467911
58	1	0	3.376671	-0.947773	-1.083258
59	6	0	2.219900	-4.312477	-2.725458
60	1	0	0.422088	-4.078583	-1.550780
61	6	0	3.490123	-3.759947	-2.988149
62	7	0	1.002961	2.427258	0.112520
63	6	0	1.595887	3.089636	-0.866576
64	6	0	0.947014	3.087207	1.374796
65	1	0	1.873382	4.133233	-0.701774
66	6	0	1.885361	2.579766	-2.210232
67	6	0	2.513685	3.462742	-3.129073
68	6	0	1.587221	1.262262	-2.645444
69	6	0	2.832567	3.045985	-4.430979
70	1	0	2.757585	4.474500	-2.810811
71	6	0	1.903527	0.846963	-3.947786
72	1	0	1.120314	0.558489	-1.958300
73	6	0	2.528261	1.734955	-4.848912
74	1	0	3.317180	3.737125	-5.115966
75	1	0	1.671236	-0.170503	-4.260020
76	1	0	2.775918	1.408438	-5.856085
77	6	0	5.209914	-1.797310	-2.851183
78	6	0	6.344392	-2.355174	-1.969040
79	1	0	6.580158	-3.398500	-2.226061
80	1	0	7.264873	-1.776340	-2.095954
81	1	0	6.080654	-2.331617	-0.899842
82	6	0	5.532664	-1.988454	-4.342685
83	1	0	5.692725	-3.043152	-4.602570
84	1	0	4.710427	-1.634063	-4.973110
85	1	0	6.434983	-1.440706	-4.629531
86	6	0	5.111577	-0.274680	-2.606011
87	1	0	4.287928	0.174287	-3.174454

88	1	0	4.960335	-0.028984	-1.549133
89	1	0	6.029613	0.233252	-2.920968
90	6	0	1.597763	-5.514759	-3.453113
91	6	0	0.663347	-4.921012	-4.529837
92	1	0	-0.115483	-4.285602	-4.094472
93	1	0	1.227409	-4.302458	-5.237983
94	1	0	0.168147	-5.704916	-5.109310
95	6	0	2.598258	-6.448153	-4.150357
96	1	0	3.287086	-6.909779	-3.436135
97	1	0	2.082269	-7.256288	-4.678449
98	1	0	3.199286	-5.906048	-4.895090
99	6	0	0.795519	-6.376743	-2.453811
100	1	0	0.366671	-7.255689	-2.942545
101	1	0	1.432871	-6.733126	-1.638599
102	1	0	-0.035288	-5.816764	-1.998820
103	6	0	-6.937452	-1.512339	0.879691
104	6	0	-3.576311	-0.134831	4.602956
105	6	0	-3.940515	1.284512	5.082252
106	1	0	-3.395056	2.045571	4.513592
107	1	0	-5.015502	1.485106	4.970876
108	1	0	-3.686664	1.420746	6.138271
109	6	0	-2.050881	-0.331314	4.747433
110	1	0	-1.743678	-1.329232	4.418534
111	1	0	-1.473908	0.399640	4.155324
112	1	0	-1.735208	-0.212572	5.788086
113	6	0	-4.252440	-1.198183	5.485067
114	1	0	-4.091262	-2.204560	5.083259
115	1	0	-3.859326	-1.178753	6.505505
116	1	0	-5.338061	-1.057452	5.548034
117	6	0	-7.948415	-0.357817	0.739365
118	1	0	-8.932616	-0.727561	0.434823
119	1	0	-8.078665	0.179134	1.690932

Anexo VI: Computational methods

120	1	0	-7.622518	0.371192	-0.009481
121	6	0	-7.466018	-2.565993	1.869442
122	1	0	-7.728347	-2.120047	2.839762
123	1	0	-8.359672	-3.067000	1.488818
124	1	0	-6.703435	-3.331044	2.079509
125	6	0	-6.791750	-2.208428	-0.493311
126	1	0	-6.575035	-1.495493	-1.296152
127	1	0	-5.981696	-2.948870	-0.487864
128	1	0	-7.714481	-2.726944	-0.771702
129	6	0	-5.868788	4.080068	-1.036560
130	6	0	-5.585037	5.160760	0.025283
131	1	0	-5.051559	4.745902	0.885873
132	1	0	-4.968741	5.974253	-0.386833
133	1	0	-6.513220	5.609798	0.392214
134	6	0	-6.741307	2.976252	-0.394115
135	1	0	-6.953229	2.174283	-1.109799
136	1	0	-6.263433	2.528402	0.484683
137	1	0	-7.703291	3.383451	-0.065771
138	6	0	-6.679420	4.663895	-2.205629
139	1	0	-7.677650	4.976666	-1.887497
140	1	0	-6.188298	5.540561	-2.650258
141	1	0	-6.795853	3.932837	-3.012600
142	6	0	-1.781099	4.036767	-4.243417
143	6	0	-1.011946	2.892190	-4.941991
144	1	0	-0.244675	2.450242	-4.293657
145	1	0	-1.686264	2.095004	-5.267259
146	1	0	-0.489233	3.260857	-5.831579
147	6	0	-2.718918	4.648866	-5.297727
148	1	0	-3.515112	3.950151	-5.574928
149	1	0	-3.215342	5.557808	-4.934653
150	1	0	-2.175765	4.918078	-6.208283
151	6	0	-0.765852	5.080805	-3.741711

152	1	0	-1.264911	5.913752	-3.224960
153	1	0	-0.048383	4.636650	-3.042239
154	1	0	-0.192980	5.507144	-4.571730
155	8	0	-4.179461	5.312370	-3.092018
156	8	0	4.349649	-4.436241	-3.864223
157	8	0	5.243920	-2.243738	4.450854
158	8	0	-6.283421	-0.894821	3.666107
159	6	0	-7.052200	0.290104	3.994192
160	1	0	-7.603796	0.631250	3.105012
161	1	0	-7.733303	-0.078239	4.768805
162	1	0	-6.388078	1.075523	4.388144
163	6	0	6.362829	-1.369172	4.153673
164	1	0	7.047829	-1.574813	4.983054
165	1	0	6.809416	-1.645235	3.186429
166	1	0	6.031277	-0.318768	4.161455
167	6	0	3.029983	-0.372176	4.983616
168	6	0	1.561925	0.049999	5.215555
169	1	0	1.142691	0.610046	4.366252
170	1	0	0.916770	-0.818694	5.382104
171	1	0	1.473460	0.696417	6.094377
172	6	0	3.485504	-1.126987	6.244161
173	1	0	4.554381	-1.377105	6.211296
174	1	0	3.317234	-0.532884	7.146844
175	1	0	2.946560	-2.072914	6.357696
176	6	0	3.882239	0.892395	4.769724
177	1	0	3.779248	1.591110	5.605252
178	1	0	4.951401	0.650985	4.675814
179	1	0	3.587347	1.419379	3.852631
180	6	0	5.267107	-4.173291	2.227911
181	6	0	4.712674	-5.328781	1.360576
182	1	0	3.831192	-5.783800	1.825063
183	1	0	4.429672	-4.995058	0.356076

184	1	0	5.460874	-6.118892	1.240993
185	6	0	5.701591	-4.792128	3.566582
186	1	0	6.215257	-4.065267	4.210315
187	1	0	4.837585	-5.150528	4.136355
188	1	0	6.382044	-5.635055	3.419284
189	6	0	6.470873	-3.544541	1.498685
190	1	0	7.251423	-4.285781	1.305511
191	1	0	6.174200	-3.106468	0.532403
192	1	0	6.923645	-2.739100	2.096985
193	6	0	5.285580	-5.322805	-3.195296
194	1	0	5.799413	-5.796806	-4.038956
195	1	0	5.986112	-4.733276	-2.583898
196	1	0	4.748045	-6.060243	-2.590261
197	6	0	-3.624947	6.494482	-2.459877
198	1	0	-4.065227	7.304693	-3.051244
199	1	0	-3.951298	6.542697	-1.409915
200	1	0	-2.527003	6.489569	-2.544988
201	1	0	0.861636	4.175223	1.328991
202	6	0	0.123298	2.405204	2.374332
203	8	0	-0.110860	1.157225	2.341619
204	8	0	-0.314439	3.081511	3.499276
205	6	0	-0.317129	4.549962	3.564090
206	1	0	-0.910170	4.975203	2.744673
207	1	0	-0.785142	4.783934	4.521617
208	1	0	0.700994	4.954807	3.543181
209	6	0	3.726934	3.416425	1.174101
210	6	0	2.747192	2.982133	2.114461
211	1	0	4.167954	2.667136	0.519838
212	1	0	2.596246	3.599951	3.003089
213	6	0	4.177456	4.765929	1.009141
214	6	0	5.184292	5.072763	0.027854
215	6	0	3.685959	5.869743	1.791205

216	6	0	5.675541	6.360159	-0.149076
217	1	0	5.574657	4.260821	-0.583074
218	6	0	4.172800	7.162467	1.622980
219	1	0	2.933445	5.692660	2.555354
220	6	0	5.171384	7.415876	0.652523
221	1	0	6.441471	6.580961	-0.884790
222	1	0	3.810223	7.989537	2.224753
223	7	0	5.681014	8.753992	0.483105
224	8	0	5.207543	9.700035	1.228065
225	8	0	6.594090	8.963191	-0.408026
226	1	0	2.757506	1.915049	2.357400

ET1b'

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	1.143170	-3.596037	-1.970784
2	6	0	0.503960	-2.841273	-0.985066
3	6	0	-0.671995	-2.142492	-1.407689
4	6	0	-1.101223	-2.201124	-2.749369
5	6	0	-0.415338	-2.957745	-3.730298
6	6	0	0.706382	-3.650279	-3.302391
7	1	0	-1.995600	-1.659251	-3.051698
8	1	0	-0.756682	-3.002721	-4.757316
9	6	0	1.045509	-2.874536	0.414026
10	6	0	1.793271	-1.819117	1.036987
11	6	0	0.917030	-4.048595	1.156659
12	6	0	2.347505	-2.000386	2.318638
13	6	0	1.468282	-4.212223	2.435626
14	6	0	2.195577	-3.204852	3.047852

15	1	0	2.926508	-1.202692	2.776137
16	1	0	2.634182	-3.333278	4.029894
17	8	0	2.278695	-4.414318	-1.803600
18	8	0	1.535760	-4.500928	-4.057200
19	8	0	1.212567	-5.510629	2.916859
20	8	0	0.270552	-5.238109	0.755836
21	6	0	2.625084	-4.917310	-3.150131
22	6	0	0.301362	-6.130207	1.934415
23	1	0	-0.712198	-6.194436	2.369974
24	1	0	0.702224	-7.099772	1.636051
25	1	0	3.572615	-4.454567	-3.477055
26	1	0	2.669253	-6.007370	-3.121364
27	15	0	-1.589614	-1.018563	-0.193681
28	15	0	1.966208	-0.162318	0.115839
29	29	0	-0.226636	0.833152	0.195524
30	6	0	-3.266724	-0.877071	-0.985912
31	6	0	-3.805632	0.382594	-1.230701
32	6	0	-3.988206	-2.027056	-1.309634
33	6	0	-5.100173	0.519902	-1.765790
34	1	0	-3.239988	1.294759	-1.005326
35	6	0	-5.298010	-1.953422	-1.796058
36	1	0	-3.537764	-3.019480	-1.168225
37	6	0	-5.854706	-0.660043	-1.942175
38	6	0	-1.966246	-2.114298	1.249902
39	6	0	-1.697130	-1.655425	2.534745
40	6	0	-2.521929	-3.379335	1.054747
41	6	0	-2.020023	-2.435365	3.660421
42	1	0	-1.224317	-0.671898	2.706257
43	6	0	-2.926405	-4.170456	2.136452
44	1	0	-2.662519	-3.763506	0.035815
45	6	0	-2.715678	-3.641095	3.432569
46	6	0	3.261702	0.756862	1.094771

47	6	0	4.506595	1.042346	0.542106
48	6	0	2.957607	1.176776	2.391352
49	6	0	5.494368	1.722504	1.274766
50	1	0	4.745644	0.749173	-0.487250
51	6	0	3.906614	1.846531	3.177531
52	1	0	1.958524	0.987868	2.815458
53	6	0	5.148430	2.158548	2.572053
54	6	0	2.969521	-0.695233	-1.362198
55	6	0	2.727920	-0.147277	-2.617829
56	6	0	3.974863	-1.646654	-1.180867
57	6	0	3.526609	-0.502625	-3.720102
58	1	0	1.919377	0.576152	-2.768356
59	6	0	4.808380	-2.028082	-2.241710
60	1	0	4.133688	-2.107100	-0.198321
61	6	0	4.607987	-1.378598	-3.480783
62	7	0	-0.518773	2.874382	0.210625
63	6	0	-0.630107	3.760678	-0.766303
64	6	0	-0.703872	3.379675	1.528260
65	6	0	-0.734471	3.471776	-2.198975
66	6	0	-0.766265	4.575112	-3.093286
67	6	0	-0.865184	2.166399	-2.739368
68	6	0	-0.924626	4.382092	-4.474751
69	1	0	-0.675278	5.583848	-2.695367
70	6	0	-1.036008	1.975539	-4.118122
71	1	0	-0.851007	1.305424	-2.073329
72	6	0	-1.064819	3.080473	-4.995253
73	1	0	-0.945936	5.240872	-5.141061
74	1	0	-1.149540	0.967111	-4.513498
75	1	0	-1.197332	2.928077	-6.063672
76	6	0	3.193045	0.072429	-5.104118
77	6	0	4.041973	1.340041	-5.321558
78	1	0	5.117926	1.118064	-5.269741

Anexo VI: Computational methods

79	1	0	3.846716	1.782652	-6.303767
80	1	0	3.823659	2.102696	-4.567233
81	6	0	3.454203	-0.957610	-6.216314
82	1	0	4.520371	-1.201042	-6.313107
83	1	0	2.935530	-1.900866	-6.011816
84	1	0	3.114436	-0.592353	-7.189482
85	6	0	1.699455	0.457310	-5.193065
86	1	0	1.054998	-0.402585	-4.981236
87	1	0	1.438520	1.262454	-4.495514
88	1	0	1.447346	0.816474	-6.196514
89	6	0	5.878233	-3.101086	-1.994379
90	6	0	5.458994	-4.033376	-0.835804
91	1	0	5.437971	-3.512937	0.128182
92	1	0	4.457238	-4.453987	-0.999133
93	1	0	6.155712	-4.870369	-0.728244
94	6	0	6.084510	-3.985983	-3.236930
95	1	0	6.549178	-3.433031	-4.064119
96	1	0	6.724792	-4.844916	-3.018559
97	1	0	5.123749	-4.360792	-3.619575
98	6	0	7.194216	-2.395580	-1.615338
99	1	0	7.981648	-3.120054	-1.385883
100	1	0	7.558472	-1.759501	-2.436039
101	1	0	7.067503	-1.750700	-0.733389
102	6	0	-3.594484	-5.523546	1.858182
103	6	0	-1.600082	-1.922280	5.046100
104	6	0	-2.762056	-1.093972	5.628742
105	1	0	-2.984905	-0.225751	4.999529
106	1	0	-3.681319	-1.691428	5.712326
107	1	0	-2.518785	-0.721238	6.628622
108	6	0	-0.351168	-1.019811	4.935701
109	1	0	0.500176	-1.568365	4.518973
110	1	0	-0.519362	-0.142554	4.288010

111	1	0	-0.053976	-0.635479	5.915525
112	6	0	-1.233015	-3.082906	5.986935
113	1	0	-0.487724	-3.741907	5.527431
114	1	0	-0.820360	-2.716571	6.930926
115	1	0	-2.098128	-3.712131	6.228115
116	6	0	-5.122356	-5.324567	1.901657
117	1	0	-5.650364	-6.267605	1.731565
118	1	0	-5.447950	-4.934295	2.877478
119	1	0	-5.459815	-4.610301	1.132119
120	6	0	-3.159998	-6.581978	2.887092
121	1	0	-3.504850	-6.332542	3.900966
122	1	0	-3.553389	-7.571893	2.642639
123	1	0	-2.063136	-6.650974	2.943388
124	6	0	-3.211702	-6.064006	0.460358
125	1	0	-3.665142	-5.473488	-0.352304
126	1	0	-2.125172	-6.062023	0.308907
127	1	0	-3.560314	-7.093319	0.328472
128	6	0	-6.051593	-3.253789	-2.109073
129	6	0	-6.895772	-3.627206	-0.874671
130	1	0	-6.258421	-3.849754	-0.002855
131	1	0	-7.574101	-2.809308	-0.589779
132	1	0	-7.511242	-4.510981	-1.068365
133	6	0	-5.074641	-4.417279	-2.401335
134	1	0	-4.385991	-4.166737	-3.214554
135	1	0	-4.477841	-4.701258	-1.519727
136	1	0	-5.623318	-5.314565	-2.708661
137	6	0	-6.942159	-3.094825	-3.352460
138	1	0	-7.416634	-4.038914	-3.633505
139	1	0	-7.744310	-2.360712	-3.191611
140	1	0	-6.364321	-2.739070	-4.211907
141	6	0	-5.611488	1.926043	-2.116073
142	6	0	-4.436070	2.865067	-2.464194

143	1	0	-3.817610	3.110853	-1.582173
144	1	0	-3.778687	2.435326	-3.227110
145	1	0	-4.801713	3.820928	-2.855800
146	6	0	-6.535872	1.896548	-3.345878
147	1	0	-6.048032	1.409984	-4.196709
148	1	0	-7.464041	1.343036	-3.156480
149	1	0	-6.819434	2.907090	-3.655223
150	6	0	-6.353813	2.490906	-0.890471
151	1	0	-7.205736	1.857418	-0.605049
152	1	0	-5.692454	2.572305	-0.020433
153	1	0	-6.743271	3.494874	-1.092601
154	8	0	-7.192298	-0.560551	-2.350599
155	8	0	5.479700	-1.679873	-4.538301
156	8	0	6.108254	2.835611	3.338361
157	8	0	-3.153119	-4.396322	4.531311
158	6	0	-4.466987	-4.016609	5.013469
159	1	0	-5.217263	-4.204175	4.230355
160	1	0	-4.606344	-4.685890	5.868954
161	1	0	-4.464516	-2.961045	5.328374
162	6	0	6.122938	4.273932	3.167005
163	1	0	6.966703	4.575126	3.797561
164	1	0	6.297538	4.535629	2.112341
165	1	0	5.178372	4.702154	3.535284
166	6	0	3.572570	2.180447	4.639857
167	6	0	2.372907	1.353573	5.152110
168	1	0	1.442861	1.582553	4.608077
169	1	0	2.554629	0.277984	5.068953
170	1	0	2.173567	1.565585	6.207581
171	6	0	4.770318	1.853823	5.550226
172	1	0	5.647681	2.470936	5.309770
173	1	0	4.530945	2.021944	6.603711
174	1	0	5.079999	0.809946	5.438998

175	6	0	3.202966	3.673020	4.745208
176	1	0	2.931664	3.937122	5.772314
177	1	0	4.042089	4.320995	4.454674
178	1	0	2.351952	3.919061	4.097019
179	6	0	6.869181	1.936422	0.623616
180	6	0	7.128819	0.898354	-0.494853
181	1	0	7.080768	-0.131652	-0.111909
182	1	0	6.403894	0.981402	-1.312596
183	1	0	8.124054	1.037702	-0.928745
184	6	0	8.005675	1.775107	1.646618
185	1	0	7.970367	2.541341	2.431594
186	1	0	7.941833	0.808886	2.158781
187	1	0	8.988092	1.841000	1.171244
188	6	0	6.894814	3.338838	-0.015415
189	1	0	7.853290	3.535315	-0.505625
190	1	0	6.106199	3.450277	-0.766430
191	1	0	6.745687	4.128820	0.735996
192	6	0	6.629105	-0.798274	-4.611895
193	1	0	7.171467	-1.191272	-5.478582
194	1	0	6.295865	0.236501	-4.787023
195	1	0	7.227559	-0.883620	-3.692110
196	6	0	-8.126769	-0.433946	-1.248083
197	1	0	-9.089455	-0.356576	-1.764705
198	1	0	-8.081266	-1.334809	-0.617592
199	1	0	-7.908571	0.478862	-0.671374
200	6	0	-0.377596	2.428903	2.592933
201	8	0	-0.245294	1.181755	2.402874
202	8	0	-0.328461	2.847579	3.911781
203	6	0	-0.178917	4.261635	4.280764
204	1	0	-0.977847	4.882749	3.864274
205	1	0	-0.236958	4.271485	5.370533
206	1	0	0.805988	4.632275	3.956692

207	1	0	-0.385004	4.413674	1.687334
208	1	0	-0.616348	4.823391	-0.514982
209	6	0	-2.636345	3.699688	1.678264
210	6	0	-3.092185	4.447988	0.552526
211	1	0	-2.643744	4.189317	2.654157
212	1	0	-3.519704	3.894906	-0.287876
213	6	0	-2.975328	5.866907	0.396446
214	6	0	-3.434628	6.501116	-0.810697
215	6	0	-2.369807	6.723660	1.380726
216	6	0	-3.290696	7.865737	-1.028802
217	1	0	-3.902809	5.882734	-1.574088
218	6	0	-2.221371	8.092060	1.172145
219	1	0	-2.030284	6.301557	2.322900
220	6	0	-2.672778	8.669863	-0.037601
221	1	0	-3.636433	8.334809	-1.943787
222	1	0	-1.763660	8.734460	1.917188
223	7	0	-2.498268	10.083877	-0.263927
224	8	0	-1.926371	10.794840	0.652613
225	8	0	-2.914669	10.590710	-1.377603
226	1	0	-2.983732	2.667042	1.735901

ET1b-endo

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-0.826043	-2.481611	-3.603963
2	6	0	-1.073410	-2.000428	-2.315565
3	6	0	-1.785116	-0.754480	-2.260068
4	6	0	-2.171735	-0.094285	-3.445282
5	6	0	-1.893415	-0.610508	-4.732760

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6	6	0	-1.219897	-1.820118	-4.774261
7	1	0	-2.729859	0.837566	-3.381338
8	1	0	-2.205657	-0.095226	-5.633289
9	6	0	-0.766585	-2.925893	-1.165134
10	6	0	0.222125	-2.801410	-0.127188
11	6	0	-1.491351	-4.124397	-1.153947
12	6	0	0.376992	-3.834844	0.824959
13	6	0	-1.313946	-5.141389	-0.208135
14	6	0	-0.386760	-5.024091	0.811789
15	1	0	1.117454	-3.732198	1.615381
16	1	0	-0.245228	-5.798842	1.555364
17	8	0	-0.154406	-3.680748	-3.939934
18	8	0	-0.830611	-2.559488	-5.910192
19	8	0	-2.189620	-6.214087	-0.459945
20	8	0	-2.507175	-4.500303	-2.065517
21	6	0	-0.377698	-3.863610	-5.388322
22	6	0	-2.843076	-5.903180	-1.744171
23	1	0	-3.925527	-5.994091	-1.628746
24	1	0	-2.435658	-6.557437	-2.522799
25	1	0	0.564839	-4.134981	-5.866032
26	1	0	-1.170956	-4.605662	-5.538506
27	15	0	-2.106609	0.052471	-0.584621
28	15	0	1.295703	-1.249773	0.110138
29	29	0	0.030415	0.655802	0.390031
30	6	0	-3.205138	1.516369	-0.971351
31	6	0	-2.655910	2.619614	-1.627266
32	6	0	-4.525640	1.553219	-0.532157
33	6	0	-3.408329	3.784628	-1.842867
34	1	0	-1.616208	2.602782	-1.978970
35	6	0	-5.318952	2.701044	-0.696064
36	1	0	-4.979434	0.687819	-0.031735
37	6	0	-4.710243	3.825688	-1.292111

38	6	0	-3.325752	-1.054280	0.258405
39	6	0	-3.350421	-1.031522	1.648328
40	6	0	-4.247888	-1.812527	-0.464310
41	6	0	-4.354566	-1.710497	2.361109
42	1	0	-2.587984	-0.474717	2.222666
43	6	0	-5.275868	-2.501072	0.193562
44	1	0	-4.179498	-1.865666	-1.555236
45	6	0	-5.343279	-2.373529	1.604121
46	6	0	2.234258	-1.670081	1.658866
47	6	0	3.360963	-2.494922	1.611350
48	6	0	1.794090	-1.150849	2.873063
49	6	0	4.099389	-2.778953	2.766965
50	1	0	3.694812	-2.925196	0.659240
51	6	0	2.493060	-1.406590	4.066485
52	1	0	0.890337	-0.518467	2.934735
53	6	0	3.683476	-2.157564	3.969621
54	6	0	2.673235	-1.325952	-1.130306
55	6	0	3.824120	-0.599548	-0.801067
56	6	0	2.607179	-2.034665	-2.322018
57	6	0	4.963560	-0.639009	-1.612178
58	1	0	3.864093	0.002848	0.116072
59	6	0	3.723429	-2.096337	-3.185339
60	1	0	1.695893	-2.567926	-2.617879
61	6	0	4.910007	-1.469909	-2.758782
62	7	0	-0.058795	2.717177	0.597126
63	6	0	0.293873	3.685160	-0.233509
64	6	0	-0.846789	3.091352	1.722126
65	1	0	-0.179636	4.670584	-0.128747
66	6	0	1.250253	3.572653	-1.335894
67	6	0	1.475221	4.716072	-2.146961
68	6	0	1.998144	2.399886	-1.612103
69	6	0	2.401035	4.684924	-3.201135

Anexo VI: Computational methods

70	1	0	0.927928	5.633884	-1.937620
71	6	0	2.922339	2.367371	-2.665587
72	1	0	1.865846	1.520371	-0.986181
73	6	0	3.128808	3.508688	-3.468023
74	1	0	2.565322	5.573991	-3.804361
75	1	0	3.491815	1.456997	-2.855375
76	1	0	3.853580	3.484294	-4.277844
77	6	0	6.186795	0.205408	-1.217103
78	6	0	7.147809	-0.681343	-0.401113
79	1	0	7.562437	-1.497222	-1.009918
80	1	0	7.993161	-0.092479	-0.026159
81	1	0	6.647781	-1.133706	0.469881
82	6	0	6.895458	0.776388	-2.456254
83	1	0	7.319898	-0.007415	-3.095146
84	1	0	6.205090	1.356246	-3.077200
85	1	0	7.714967	1.445036	-2.167816
86	6	0	5.764265	1.404493	-0.345505
87	1	0	5.033787	2.043688	-0.855073
88	1	0	5.341953	1.097369	0.615571
89	1	0	6.627628	2.054488	-0.116542
90	6	0	3.509132	-2.779694	-4.543811
91	6	0	2.461172	-1.935489	-5.304140
92	1	0	1.505234	-1.880706	-4.774530
93	1	0	2.815328	-0.906708	-5.440096
94	1	0	2.261281	-2.342295	-6.299513
95	6	0	4.755632	-2.869132	-5.437097
96	1	0	5.488047	-3.583210	-5.051799
97	1	0	4.495042	-3.186540	-6.451535
98	1	0	5.263797	-1.896905	-5.517090
99	6	0	2.988669	-4.212735	-4.302609
100	1	0	2.883512	-4.759921	-5.243184
101	1	0	3.678064	-4.779309	-3.668761

102	1	0	2.010438	-4.214073	-3.802753
103	6	0	-6.267427	-3.339303	-0.625875
104	6	0	-4.308112	-1.656405	3.895773
105	6	0	-5.146648	-0.446000	4.357002
106	1	0	-4.720331	0.491314	3.981557
107	1	0	-6.184977	-0.513745	4.003455
108	1	0	-5.172953	-0.380117	5.449256
109	6	0	-2.858071	-1.460649	4.391254
110	1	0	-2.213718	-2.286947	4.074197
111	1	0	-2.407685	-0.527344	4.012592
112	1	0	-2.817801	-1.408254	5.483339
113	6	0	-4.826265	-2.957761	4.529404
114	1	0	-4.305774	-3.829412	4.116422
115	1	0	-4.677100	-2.961352	5.613020
116	1	0	-5.893718	-3.119337	4.343941
117	6	0	-7.578191	-2.544919	-0.792791
118	1	0	-8.305745	-3.105963	-1.387840
119	1	0	-8.048857	-2.330793	0.177355
120	1	0	-7.403646	-1.588419	-1.295077
121	6	0	-6.527779	-4.687163	0.068711
122	1	0	-7.011016	-4.550054	1.048138
123	1	0	-7.178020	-5.331935	-0.527105
124	1	0	-5.592211	-5.223035	0.258654
125	6	0	-5.722654	-3.643960	-2.040586
126	1	0	-5.672911	-2.745876	-2.665269
127	1	0	-4.712445	-4.069336	-2.000010
128	1	0	-6.366418	-4.358474	-2.562193
129	6	0	-6.773075	2.668281	-0.204139
130	6	0	-6.804144	3.228289	1.233028
131	1	0	-6.200858	2.618076	1.911785
132	1	0	-6.418211	4.257932	1.267920
133	1	0	-7.825860	3.250756	1.625609

134	6	0	-7.319754	1.221387	-0.181474
135	1	0	-7.304467	0.779349	-1.183981
136	1	0	-6.740723	0.565926	0.480199
137	1	0	-8.356677	1.201664	0.168353
138	6	0	-7.700414	3.479018	-1.123976
139	1	0	-8.749957	3.368125	-0.838000
140	1	0	-7.467261	4.551835	-1.106337
141	1	0	-7.600022	3.160261	-2.167351
142	6	0	-2.783891	4.937831	-2.642636
143	6	0	-1.695227	4.412014	-3.604556
144	1	0	-0.868568	3.920363	-3.076096
145	1	0	-2.107410	3.696384	-4.322723
146	1	0	-1.253209	5.231580	-4.181872
147	6	0	-3.834595	5.652502	-3.509861
148	1	0	-4.376992	4.941954	-4.142453
149	1	0	-4.590321	6.169798	-2.904558
150	1	0	-3.373772	6.399175	-4.163035
151	6	0	-2.139681	5.924362	-1.649301
152	1	0	-2.887505	6.354115	-0.966976
153	1	0	-1.370746	5.435551	-1.032829
154	1	0	-1.661712	6.757954	-2.174100
155	8	0	-5.455282	5.008799	-1.407910
156	8	0	6.066149	-1.613544	-3.536728
157	8	0	4.448864	-2.367571	5.124804
158	8	0	-6.400070	-3.013330	2.269490
159	6	0	-7.525101	-2.150283	2.568781
160	1	0	-8.009769	-1.841449	1.630128
161	1	0	-8.177003	-2.808929	3.152973
162	1	0	-7.200521	-1.281344	3.161748
163	6	0	5.449317	-1.343540	5.360370
164	1	0	5.898080	-1.667673	6.305344
165	1	0	6.187412	-1.350205	4.543624

166	1	0	4.967496	-0.358500	5.463062
167	6	0	1.932905	-0.839976	5.380431
168	6	0	0.402351	-0.656272	5.290033
169	1	0	0.102701	0.003121	4.458652
170	1	0	-0.105581	-1.614762	5.142970
171	1	0	0.003783	-0.209335	6.205581
172	6	0	2.198600	-1.786949	6.563609
173	1	0	3.266929	-1.870340	6.797660
174	1	0	1.691346	-1.444584	7.470054
175	1	0	1.848321	-2.801189	6.344876
176	6	0	2.584514	0.535092	5.624454
177	1	0	2.232685	0.980045	6.560507
178	1	0	3.680100	0.458080	5.688346
179	1	0	2.350072	1.237161	4.817147
180	6	0	5.310248	-3.717370	2.665434
181	6	0	5.191200	-4.650708	1.436890
182	1	0	4.287205	-5.265973	1.490492
183	1	0	5.167064	-4.093528	0.494056
184	1	0	6.045572	-5.333786	1.384576
185	6	0	5.419955	-4.622948	3.903725
186	1	0	5.611299	-4.045518	4.819172
187	1	0	4.491080	-5.176558	4.074907
188	1	0	6.231327	-5.348521	3.801028
189	6	0	6.575461	-2.854470	2.503641
190	1	0	7.470664	-3.473716	2.396147
191	1	0	6.509823	-2.201887	1.616762
192	1	0	6.731826	-2.202316	3.376207
193	6	0	6.905652	-2.721181	-3.116371
194	1	0	7.691079	-2.720108	-3.880340
195	1	0	7.323579	-2.508192	-2.119125
196	1	0	6.339684	-3.656355	-3.122803
197	6	0	-5.287511	5.917798	-0.291308

198	1	0	-5.939661	6.753302	-0.569544
199	1	0	-5.628838	5.438626	0.638374
200	1	0	-4.236875	6.240222	-0.223853
201	1	0	-1.554177	3.906410	1.547924
202	6	0	-1.343286	1.965534	2.517641
203	8	0	-0.822915	0.808272	2.503958
204	8	0	-2.354845	2.167929	3.448668
205	6	0	-3.243308	3.334988	3.374699
206	1	0	-3.761439	3.368162	2.405857
207	1	0	-3.967016	3.183733	4.177197
208	1	0	-2.697588	4.269936	3.543039
209	6	0	1.043766	5.105742	2.291956
210	6	0	0.333887	4.069549	2.960590
211	1	0	0.520701	6.050781	2.137820
212	1	0	-0.445637	4.386679	3.655676
213	6	0	2.402363	5.054885	1.838006
214	6	0	2.981105	6.207695	1.201263
215	6	0	3.264186	3.917937	2.019419
216	6	0	4.300393	6.228801	0.767896
217	1	0	2.358172	7.089462	1.059540
218	6	0	4.587324	3.933924	1.598436
219	1	0	2.876744	3.023402	2.499403
220	6	0	5.115852	5.085801	0.962515
221	1	0	4.725972	7.100635	0.282330
222	1	0	5.237975	3.079287	1.749551
223	7	0	6.479108	5.091569	0.508379
224	8	0	7.203456	4.029528	0.689339
225	8	0	6.943687	6.151063	-0.068998
226	1	0	0.909049	3.226339	3.345072

ET2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.481309	1.995169	-3.757939
2	6	0	-0.985306	1.907688	-2.454586
3	6	0	0.374372	1.458486	-2.349876
4	6	0	1.111263	1.133681	-3.509076
5	6	0	0.569905	1.227965	-4.812672
6	6	0	-0.739080	1.671746	-4.900603
7	1	0	2.149354	0.820957	-3.414071
8	1	0	1.155141	0.983558	-5.691283
9	6	0	-1.829447	2.503765	-1.356950
10	6	0	-2.485132	1.865613	-0.246537
11	6	0	-2.071778	3.878096	-1.482006
12	6	0	-3.264814	2.640406	0.643733
13	6	0	-2.864889	4.621344	-0.600144
14	6	0	-3.470039	4.030806	0.494348
15	1	0	-3.745292	2.165195	1.496014
16	1	0	-4.073673	4.594467	1.195273
17	8	0	-2.779919	2.412765	-4.138825
18	8	0	-1.514774	1.870986	-6.062091
19	8	0	-2.913168	5.972825	-0.991098
20	8	0	-1.559140	4.733708	-2.487485
21	6	0	-2.718183	2.590546	-5.603348
22	6	0	-2.249082	6.027210	-2.306249
23	1	0	-1.507431	6.829152	-2.303044
24	1	0	-3.008553	6.143736	-3.088124
25	1	0	-3.601709	2.140347	-6.057898
26	1	0	-2.607352	3.657716	-5.831211
27	15	0	1.135299	1.194674	-0.638377

28	15	0	-2.297210	0.009778	0.156744
29	29	0	-0.110787	-0.655295	0.431377
30	6	0	2.905568	0.715674	-1.013409
31	6	0	3.153440	-0.519927	-1.614147
32	6	0	3.968082	1.539424	-0.651631
33	6	0	4.462533	-0.950351	-1.880181
34	1	0	2.324426	-1.184090	-1.888569
35	6	0	5.300446	1.142722	-0.851708
36	1	0	3.789891	2.518301	-0.189445
37	6	0	5.519550	-0.134909	-1.412418
38	6	0	1.411046	2.895906	0.044788
39	6	0	1.535698	2.999928	1.427178
40	6	0	1.596764	4.004423	-0.779241
41	6	0	1.945002	4.204816	2.022652
42	1	0	1.326430	2.137594	2.080985
43	6	0	1.998305	5.234825	-0.237781
44	1	0	1.442115	3.920587	-1.859680
45	6	0	2.237097	5.282131	1.157534
46	6	0	-3.253259	-0.094930	1.755851
47	6	0	-4.651882	-0.125105	1.750404
48	6	0	-2.558321	-0.095394	2.961061
49	6	0	-5.379920	-0.200255	2.943164
50	1	0	-5.204158	-0.093853	0.803434
51	6	0	-3.238158	-0.166738	4.191903
52	1	0	-1.455738	-0.042635	2.989608
53	6	0	-4.640173	-0.302301	4.147256
54	6	0	-3.463248	-0.906737	-0.965462
55	6	0	-3.989352	-2.107668	-0.470844
56	6	0	-3.809346	-0.459214	-2.233112
57	6	0	-4.965283	-2.815753	-1.179794
58	1	0	-3.664171	-2.499458	0.500256
59	6	0	-4.753941	-1.163086	-3.012636

Anexo VI: Computational methods

60	1	0	-3.367287	0.449917	-2.658074
61	6	0	-5.390681	-2.265903	-2.415364
62	7	0	1.278815	-2.032846	0.844356
63	6	0	1.706480	-3.160852	0.199087
64	6	0	2.201562	-1.744052	1.928863
65	1	0	2.770949	-3.219515	-0.099049
66	6	0	0.805178	-3.950574	-0.670344
67	6	0	1.353768	-4.791933	-1.669193
68	6	0	-0.601542	-3.931012	-0.504263
69	6	0	0.523695	-5.574230	-2.490813
70	1	0	2.433933	-4.832377	-1.800665
71	6	0	-1.430288	-4.712038	-1.324878
72	1	0	-1.029315	-3.309564	0.278891
73	6	0	-0.874572	-5.535518	-2.325616
74	1	0	0.964365	-6.210788	-3.254249
75	1	0	-2.514601	-4.685379	-1.178581
76	1	0	-1.519773	-6.138517	-2.960414
77	6	0	-5.532750	-4.121331	-0.603289
78	6	0	-6.867456	-3.811805	0.100183
79	1	0	-7.604494	-3.389997	-0.598635
80	1	0	-7.308011	-4.717988	0.527626
81	1	0	-6.734945	-3.085986	0.919924
82	6	0	-5.736248	-5.164880	-1.715396
83	1	0	-6.499616	-4.845622	-2.440001
84	1	0	-4.815073	-5.328410	-2.283813
85	1	0	-6.056027	-6.128720	-1.309670
86	6	0	-4.571704	-4.742710	0.434178
87	1	0	-3.590619	-4.963211	-0.016083
88	1	0	-4.408434	-4.090302	1.297904
89	1	0	-4.967484	-5.689178	0.817674
90	6	0	-4.958296	-0.688372	-4.458726
91	6	0	-3.575213	-0.712337	-5.147974

Anexo VI: Computational methods

92	1	0	-2.854865	-0.044212	-4.665918
93	1	0	-3.146453	-1.721186	-5.127052
94	1	0	-3.642996	-0.410825	-6.197520
95	6	0	-5.891009	-1.571534	-5.302832
96	1	0	-6.944349	-1.423538	-5.053015
97	1	0	-5.782615	-1.356919	-6.370880
98	1	0	-5.674064	-2.639012	-5.157559
99	6	0	-5.526311	0.745391	-4.425214
100	1	0	-5.753048	1.105001	-5.432712
101	1	0	-6.452200	0.791818	-3.844128
102	1	0	-4.819523	1.451269	-3.968049
103	6	0	2.172869	6.441631	-1.170972
104	6	0	2.075124	4.250626	3.552729
105	6	0	3.533339	3.900892	3.917824
106	1	0	3.790454	2.890485	3.582702
107	1	0	4.244964	4.601641	3.458076
108	1	0	3.686941	3.939738	5.000816
109	6	0	1.146024	3.210560	4.217577
110	1	0	0.097278	3.390319	3.959737
111	1	0	1.388422	2.177841	3.917595
112	1	0	1.228938	3.247954	5.307947
113	6	0	1.684231	5.626973	4.115066
114	1	0	0.683813	5.919674	3.777145
115	1	0	1.682059	5.626688	5.208730
116	1	0	2.366047	6.420757	3.787231
117	6	0	3.666695	6.585046	-1.524014
118	1	0	3.833544	7.432895	-2.195993
119	1	0	4.280824	6.754247	-0.627507
120	1	0	4.047287	5.687010	-2.020827
121	6	0	1.639030	7.723337	-0.508914
122	1	0	2.212701	7.985754	0.392192
123	1	0	1.687092	8.579437	-1.186256

124	1	0	0.599393	7.599384	-0.187531
125	6	0	1.391452	6.249264	-2.491599
126	1	0	1.810473	5.445659	-3.106821
127	1	0	0.341173	5.999185	-2.299296
128	1	0	1.415910	7.160105	-3.097103
129	6	0	6.429056	2.100745	-0.443664
130	6	0	6.911249	1.700870	0.965960
131	1	0	6.109559	1.792985	1.703442
132	1	0	7.271285	0.660553	0.982763
133	1	0	7.741626	2.334604	1.293534
134	6	0	5.933366	3.565816	-0.394377
135	1	0	5.572624	3.893096	-1.375751
136	1	0	5.118194	3.706444	0.324793
137	1	0	6.744936	4.240146	-0.103619
138	6	0	7.591232	2.057893	-1.449112
139	1	0	8.353528	2.806818	-1.218754
140	1	0	8.088967	1.077770	-1.462080
141	1	0	7.239201	2.236606	-2.470652
142	6	0	4.672042	-2.261034	-2.654801
143	6	0	3.438598	-2.579265	-3.533145
144	1	0	2.524471	-2.709143	-2.942458
145	1	0	3.256644	-1.788185	-4.266993
146	1	0	3.591122	-3.509422	-4.092040
147	6	0	5.876546	-2.160929	-3.606147
148	1	0	5.789715	-1.298205	-4.273554
149	1	0	6.824176	-2.042587	-3.063004
150	1	0	5.972863	-3.058992	-4.223929
151	6	0	4.872099	-3.401560	-1.643733
152	1	0	5.794408	-3.272363	-1.055383
153	1	0	4.041558	-3.466301	-0.920558
154	1	0	4.956663	-4.373676	-2.141269
155	8	0	6.840260	-0.565004	-1.590375

156	8	0	-6.447480	-2.895213	-3.088593
157	8	0	-5.350616	-0.463232	5.345297
158	8	0	2.706996	6.484194	1.708457
159	6	0	4.148677	6.553967	1.839085
160	1	0	4.613993	6.530632	0.841527
161	1	0	4.293359	7.526780	2.321355
162	1	0	4.515920	5.734124	2.475617
163	6	0	-5.484302	-1.845501	5.763841
164	1	0	-6.003184	-1.750368	6.723860
165	1	0	-6.096229	-2.393887	5.031786
166	1	0	-4.491095	-2.304325	5.889818
167	6	0	-2.417960	-0.102336	5.489889
168	6	0	-1.116971	0.699929	5.274440
169	1	0	-0.482905	0.274725	4.479951
170	1	0	-1.328421	1.737772	4.997122
171	1	0	-0.509605	0.720210	6.184336
172	6	0	-3.191068	0.603350	6.617697
173	1	0	-4.057699	0.024428	6.956990
174	1	0	-2.553553	0.776613	7.489664
175	1	0	-3.576160	1.573604	6.285898
176	6	0	-2.056292	-1.544249	5.896918
177	1	0	-1.483404	-1.560150	6.829551
178	1	0	-2.956072	-2.157446	6.051480
179	1	0	-1.448375	-2.034582	5.128998
180	6	0	-6.913924	-0.165926	2.894649
181	6	0	-7.418483	0.471729	1.578501
182	1	0	-7.057125	1.499814	1.470128
183	1	0	-7.101764	-0.093339	0.695393
184	1	0	-8.512812	0.510827	1.560914
185	6	0	-7.481826	0.677875	4.048650
186	1	0	-7.259862	0.231665	5.028989
187	1	0	-7.047568	1.682783	4.058621

188	1	0	-8.567797	0.781173	3.976249
189	6	0	-7.438173	-1.612001	2.967997
190	1	0	-8.531547	-1.640857	2.945768
191	1	0	-7.068301	-2.216049	2.122767
192	1	0	-7.116329	-2.110021	3.894458
193	6	0	-7.737577	-2.287100	-2.816286
194	1	0	-8.398042	-2.818176	-3.510838
195	1	0	-8.017533	-2.489166	-1.770253
196	1	0	-7.714896	-1.214214	-3.024903
197	6	0	7.357746	-1.375135	-0.504029
198	1	0	8.366801	-1.620645	-0.856525
199	1	0	7.390108	-0.781938	0.420766
200	1	0	6.752503	-2.288422	-0.385918
201	1	0	3.249873	-1.647921	1.581119
202	6	0	1.801956	-0.491812	2.689966
203	8	0	0.670654	0.033136	2.608941
204	8	0	2.700321	0.106157	3.550356
205	6	0	4.125470	-0.261242	3.611109
206	1	0	4.610945	-0.091787	2.641769
207	1	0	4.547194	0.410172	4.360326
208	1	0	4.256656	-1.299822	3.929265
209	6	0	2.235267	-4.279151	2.001086
210	6	0	2.158453	-3.054008	2.877918
211	1	0	1.360882	-4.926385	1.998937
212	1	0	2.962789	-3.017226	3.622936
213	6	0	3.489861	-4.904021	1.679696
214	6	0	3.526563	-6.198704	1.057673
215	6	0	4.751816	-4.236704	1.851149
216	6	0	4.717440	-6.780270	0.637413
217	1	0	2.589582	-6.732682	0.914731
218	6	0	5.949974	-4.810033	1.435350
219	1	0	4.782650	-3.265833	2.337382

220	6	0	5.937595	-6.080710	0.818073
221	1	0	4.737499	-7.759804	0.171920
222	1	0	6.900795	-4.307925	1.575638
223	7	0	7.179709	-6.666432	0.371812
224	8	0	8.272696	-5.991324	0.524738
225	8	0	7.155883	-7.835935	-0.172003
226	1	0	1.201652	-3.023114	3.409360

Table VI.2. Total electronic energies^a (E, in a.u.), thermal corrections to Gibbs free energies^b (TCGFE, in a.u.), and number of imaginary frequencies^c (NIMAG) of all stationary points discussed in the main text corresponding to the dipolar cycloaddition of *p*-nitrobenzene **59a** with azomethine ylide derived from imine **48a** and Ag/(*R*)-Fesulphos as catalytic system.

Structure	E	T	NIMAG(ν)
INT1d	-1884.812880	0.557373	0
INT1d'	-1884.804567	0.556061	0
INT2d	-2398.842753	0.686237	0
INT3d	-2398.848927	0.687026	0
<i>endo-64a</i>	-1106.764790	0.282875	0
ET1d	-2398.838331	0.682198	1 (-343.7360)
ET1d'	-2398.843925	0.683483	1 (-353.5275)
ET1d-<i>exo</i>	-2398.828065	0.681516	1 (-350.6944)
ET2d	-2398.844030	0.687291	1 (-204.9937)

^aComputed at M06L/LANL2DZ// B3LYP/LANL2DZ level of theory. ^b Computed at 298.15 K B3LYP/LANL2DZ level of theory. ^cIf NIMAG=1, the imaginary frequency ν (in parentheses) is given in cm⁻¹.

Cartesian of all the stationary collected in Table VI.2.

INT1d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.999416	4.176048	-0.820615
2	7	0	1.873145	3.132156	-0.613972
3	6	0	3.167231	3.332950	-0.407686
4	6	0	4.192852	2.294563	-0.328429
5	6	0	4.039998	0.993340	-0.880839
6	6	0	5.073112	0.045504	-0.798301
7	6	0	6.294644	0.368961	-0.171970
8	6	0	6.471537	1.662748	0.361728
9	6	0	5.439851	2.610538	0.279768
10	15	0	0.497442	-1.317417	0.162818
11	6	0	1.400768	-1.938576	1.697331
12	6	0	0.790889	-2.809542	2.623663
13	6	0	1.504275	-3.251009	3.754396
14	6	0	2.829970	-2.827156	3.965444
15	6	0	3.438265	-1.951294	3.044855
16	6	0	2.725247	-1.503340	1.917999
17	6	0	-0.371558	3.929115	-1.016552
18	8	0	-1.106800	5.089448	-1.293050
19	6	0	-2.531248	4.927070	-1.580729
20	8	0	-0.976251	2.784100	-0.970742
21	6	0	-1.260200	-1.812980	0.471157
22	6	0	-1.952231	-3.013711	0.046421
23	6	0	-3.300774	-2.945377	0.543322
24	6	0	-3.447062	-1.719034	1.289906
25	6	0	-2.186241	-1.024696	1.273634
26	26	0	-2.907019	-1.328354	-0.749869
27	6	0	-4.296940	-0.025536	-1.698017
28	6	0	-4.402143	-1.353634	-2.252394
29	6	0	-3.122573	-1.696836	-2.822888

30	6	0	-2.235234	-0.578216	-2.618839
31	6	0	-2.957429	0.458231	-1.925432
32	16	0	-1.569312	0.379565	2.264479
33	6	0	-3.012863	1.660093	2.582013
34	6	0	-4.001068	1.082040	3.615439
35	6	0	1.085462	-2.498402	-1.182948
36	6	0	1.329381	-1.987441	-2.474637
37	6	0	1.780670	-2.834664	-3.504539
38	6	0	1.995845	-4.201870	-3.247810
39	6	0	1.764845	-4.715375	-1.956069
40	6	0	1.313590	-3.867815	-0.927560
41	6	0	-2.248476	2.866070	3.172087
42	6	0	-3.701681	2.041141	1.264038
43	1	0	-4.343452	-1.399524	1.798544
44	1	0	-4.076319	-3.680597	0.378954
45	1	0	-1.532722	-3.802220	-0.560631
46	1	0	-2.537509	1.406020	-1.615077
47	1	0	-1.204757	-0.524741	-2.936576
48	1	0	-5.091922	0.511336	-1.199536
49	1	0	-5.281556	-1.982892	-2.236195
50	1	0	-2.870104	-2.629854	-3.307607
51	1	0	5.586515	3.606320	0.695245
52	1	0	7.412944	1.929957	0.837209
53	1	0	4.934939	-0.939169	-1.240654
54	1	0	3.124759	0.746846	-1.412368
55	1	0	-4.446106	2.826710	1.465459
56	1	0	-2.971847	2.417597	0.540514
57	1	0	-4.218982	1.185596	0.821145
58	1	0	-4.747515	1.848657	3.871079
59	1	0	-4.538304	0.210762	3.226094
60	1	0	-3.485185	0.783011	4.534781
61	1	0	-2.970735	3.646972	3.447486

62	1	0	-1.688365	2.590306	4.074572
63	1	0	-1.548550	3.285775	2.441231
64	1	0	-0.236611	-3.131208	2.478050
65	1	0	1.024012	-3.917300	4.467158
66	1	0	3.379262	-3.167147	4.840342
67	1	0	4.457599	-1.608897	3.204688
68	1	0	3.201943	-0.814645	1.224838
69	1	0	1.183824	-0.927863	-2.675104
70	1	0	1.968949	-2.427192	-4.494715
71	1	0	2.349136	-4.857208	-4.040352
72	1	0	1.941766	-5.767939	-1.748273
73	1	0	1.163473	-4.269013	0.071401
74	1	0	-3.066084	4.534548	-0.708178
75	1	0	-2.885362	5.931764	-1.823083
76	1	0	-2.686072	4.250398	-2.428960
77	1	0	1.362023	5.199452	-0.880664
78	1	0	3.524778	4.364498	-0.306006
79	1	0	7.095820	-0.364161	-0.116772
80	47	0	0.719953	1.167991	-0.322956

INT1d'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.625434	3.100483	0.009477
2	7	0	2.283933	3.095774	-0.302278
3	6	0	1.600470	4.231073	-0.390780
4	6	0	0.227524	4.397803	-0.853457
5	6	0	-0.498241	3.417922	-1.584345
6	6	0	-1.797299	3.677165	-2.048535

7	6	0	-2.416678	4.919088	-1.798602
8	6	0	-1.710758	5.905259	-1.079096
9	6	0	-0.410008	5.650211	-0.620598
10	15	0	0.635196	-1.428651	-0.144580
11	6	0	1.681157	-2.420224	1.072626
12	6	0	1.134474	-3.455828	1.860255
13	6	0	1.955464	-4.180563	2.744473
14	6	0	3.326373	-3.875864	2.845731
15	6	0	3.868300	-2.833974	2.068774
16	6	0	3.052034	-2.098911	1.187610
17	6	0	4.360043	1.901894	0.111899
18	8	0	5.719473	2.118804	0.378088
19	6	0	6.565693	0.931937	0.495282
20	8	0	3.920142	0.696097	-0.017151
21	6	0	-1.096840	-1.848068	0.374016
22	6	0	-1.857991	-3.018650	-0.019208
23	6	0	-3.093759	-3.014115	0.712505
24	6	0	-3.109679	-1.846508	1.561914
25	6	0	-1.872960	-1.128587	1.373909
26	26	0	-2.944461	-1.283551	-0.477426
27	6	0	-4.675490	-0.185516	-1.012934
28	6	0	-4.533064	-1.329428	-1.881395
29	6	0	-3.271166	-1.211610	-2.571156
30	6	0	-2.638737	0.007536	-2.128972
31	6	0	-3.503842	0.641482	-1.166100
32	16	0	-1.183135	0.336449	2.219471
33	6	0	-2.543954	1.027598	3.431983
34	6	0	-2.838790	-0.002035	4.541770
35	6	0	0.840761	-2.363355	-1.769431
36	6	0	0.746345	-1.645048	-2.979761
37	6	0	0.889545	-2.304829	-4.214504
38	6	0	1.136763	-3.690682	-4.248139

39	6	0	1.247129	-4.409805	-3.042118
40	6	0	1.100035	-3.749642	-1.807687
41	6	0	-1.847415	2.271381	4.029900
42	6	0	-3.806370	1.445646	2.653444
43	1	0	-3.918063	-1.573885	2.220880
44	1	0	-3.884928	-3.746372	0.632524
45	1	0	-1.545280	-3.754434	-0.745128
46	1	0	-3.295734	1.563819	-0.644836
47	1	0	-1.677126	0.376654	-2.453327
48	1	0	-5.513435	0.013390	-0.359149
49	1	0	-5.242550	-2.138308	-1.988765
50	1	0	-2.865681	-1.915825	-3.283968
51	1	0	0.130523	6.421247	-0.073554
52	1	0	-2.171836	6.871323	-0.884279
53	1	0	-2.324392	2.922819	-2.627378
54	1	0	-0.019731	2.469438	-1.820250
55	1	0	-4.541104	1.867613	3.354719
56	1	0	-3.564868	2.212266	1.908809
57	1	0	-4.275211	0.604249	2.134895
58	1	0	-3.553486	0.429298	5.258182
59	1	0	-3.270660	-0.928045	4.151079
60	1	0	-1.922304	-0.261148	5.083280
61	1	0	-2.526209	2.749987	4.748893
62	1	0	-0.925750	2.001000	4.558958
63	1	0	-1.599128	3.004350	3.253558
64	1	0	0.075835	-3.691031	1.801709
65	1	0	1.524739	-4.973624	3.351398
66	1	0	3.960971	-4.435222	3.529529
67	1	0	4.922476	-2.581381	2.154047
68	1	0	3.480189	-1.272199	0.624394
69	1	0	0.583978	-0.569446	-2.961816
70	1	0	0.821763	-1.738649	-5.140164

71	1	0	1.256108	-4.200907	-5.200970
72	1	0	1.454618	-5.477049	-3.060297
73	1	0	1.212199	-4.308911	-0.882687
74	1	0	6.529909	0.333088	-0.421764
75	1	0	7.573064	1.320012	0.663341
76	1	0	6.249133	0.308652	1.340271
77	1	0	4.150362	4.043060	0.144455
78	1	0	2.119288	5.158611	-0.122381
79	1	0	-3.419648	5.117428	-2.168699
80	47	0	1.486355	0.968681	-0.275092

INT2d

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	0.650947	-3.145688	0.911096
2	6	0	1.184497	-3.611908	-0.342360
3	6	0	0.500152	-4.830955	-0.684617
4	6	0	-0.448173	-5.129016	0.361660
5	6	0	-0.356350	-4.084822	1.351942
6	26	0	-0.934003	-3.270170	-0.511013
7	6	0	-1.391655	-1.670867	-1.833588
8	6	0	-2.164359	-1.541122	-0.605415
9	6	0	-2.979197	-2.729791	-0.472055
10	6	0	-2.721948	-3.580333	-1.605047
11	6	0	-1.737175	-2.936715	-2.436656
12	15	0	-2.217388	-0.041432	0.478059
13	6	0	-3.654342	0.955452	-0.222179

14	6	0	-4.765956	0.332712	-0.830315
15	6	0	-5.830122	1.108095	-1.325047
16	6	0	-5.791528	2.512512	-1.217718
17	6	0	-4.678280	3.136203	-0.623981
18	6	0	-3.608742	2.362650	-0.131444
19	16	0	-0.172061	-0.469013	-2.456401
20	6	0	-0.991708	0.285991	-4.074676
21	6	0	-0.024130	1.427080	-4.452911
22	47	0	-0.136801	1.369602	0.729073
23	7	0	1.568004	2.653114	1.371789
24	6	0	1.716580	3.947718	0.720291
25	6	0	0.382416	4.545954	0.366561
26	8	0	0.471656	5.910118	0.240809
27	6	0	-0.731676	6.639608	-0.203345
28	6	0	2.631972	2.240078	2.029269
29	6	0	2.745595	0.949698	2.721119
30	6	0	1.637626	0.333095	3.354910
31	6	0	1.800275	-0.881573	4.041137
32	6	0	3.062275	-1.508023	4.089855
33	6	0	4.167544	-0.901715	3.460757
34	6	0	4.014797	0.324886	2.794692
35	6	0	2.622769	3.820953	-0.656661
36	6	0	3.919489	3.128447	-0.462775
37	6	0	4.175901	1.781525	-0.790883
38	6	0	3.169696	0.882657	-1.320315
39	6	0	3.445046	-0.445787	-1.592857
40	6	0	4.744376	-0.973881	-1.364209
41	6	0	5.777716	-0.115779	-0.886331
42	6	0	5.499487	1.211835	-0.611283
43	7	0	5.000439	-2.351087	-1.599341
44	8	0	6.202393	-2.815394	-1.434167
45	8	0	-0.676896	3.918960	0.134631

46	6	0	-2.879786	-0.692306	2.121287
47	6	0	-1.965991	-1.290091	3.016815
48	6	0	-2.401546	-1.770805	4.264247
49	6	0	-3.755362	-1.650868	4.635549
50	6	0	-4.667166	-1.046452	3.750887
51	6	0	-4.232741	-0.569590	2.498178
52	8	0	4.011626	-3.126133	-1.964990
53	6	0	-1.029433	-0.791108	-5.175776
54	6	0	-2.398565	0.819804	-3.762677
55	1	0	-1.301430	-3.335678	-3.340334
56	1	0	-3.171229	-4.546709	-1.786001
57	1	0	-3.654550	-2.940788	0.345099
58	1	0	1.981610	-3.161530	-0.919546
59	1	0	0.982155	-2.263720	1.441101
60	1	0	0.674136	-5.417536	-1.575908
61	1	0	-1.119958	-5.976094	0.391482
62	1	0	-0.946317	-4.016486	2.254996
63	1	0	4.866659	0.782466	2.297950
64	1	0	5.140311	-1.385447	3.484157
65	1	0	0.953372	-1.330575	4.555080
66	1	0	0.671557	0.833227	3.355227
67	1	0	-1.383551	-0.340780	-6.115045
68	1	0	-0.034985	-1.216549	-5.350947
69	1	0	-1.717144	-1.603643	-4.916761
70	1	0	-2.835895	1.249205	-4.676401
71	1	0	-3.063524	0.021312	-3.415637
72	1	0	-2.371021	1.600522	-2.994728
73	1	0	-0.365795	1.895024	-5.386506
74	1	0	0.004587	2.199632	-3.674962
75	1	0	0.995576	1.056453	-4.613034
76	1	0	-4.798252	-0.748198	-0.934509
77	1	0	-6.680873	0.619219	-1.793592

78	1	0	-6.614158	3.111660	-1.601038
79	1	0	-4.633299	4.220123	-0.552142
80	1	0	-2.741004	2.860956	0.291693
81	1	0	-0.917937	-1.376854	2.745504
82	1	0	-1.689398	-2.231584	4.945039
83	1	0	-4.091454	-2.016722	5.602659
84	1	0	-5.712324	-0.941667	4.031709
85	1	0	-4.947183	-0.095437	1.832286
86	1	0	-1.528801	6.532367	0.538972
87	1	0	-0.412504	7.678866	-0.286565
88	1	0	-1.072703	6.252525	-1.168484
89	1	0	2.260069	4.663479	1.349675
90	1	0	3.501580	2.897511	2.096768
91	1	0	3.183367	-2.452683	4.613939
92	1	0	2.759276	4.863332	-0.969506
93	1	0	1.988784	3.321461	-1.398405
94	1	0	4.751260	3.730501	-0.096206
95	1	0	2.166356	1.249503	-1.514173
96	1	0	6.295181	1.862974	-0.250974
97	1	0	2.677260	-1.096725	-1.995041
98	1	0	6.771010	-0.529263	-0.743690

INT3d

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-1.928375	3.565634	-1.404331
2	7	0	-1.466552	2.257042	-1.842053
3	6	0	-2.663158	1.694643	-2.470388
4	6	0	-2.481606	0.299783	-3.055946

5	6	0	-1.285885	0.025835	-3.764876
6	6	0	-1.097485	-1.199793	-4.428116
7	6	0	-2.102883	-2.186284	-4.398035
8	6	0	-3.298715	-1.922730	-3.706235
9	6	0	-3.487011	-0.691039	-3.049066
10	15	0	2.329669	0.153800	-0.333838
11	6	0	3.564646	1.345637	0.439986
12	6	0	4.649192	0.902705	1.227578
13	6	0	5.555863	1.830216	1.772069
14	6	0	5.384325	3.208674	1.535619
15	6	0	4.294899	3.654426	0.763558
16	6	0	3.383562	2.727761	0.221302
17	6	0	-0.992620	4.275204	-0.448626
18	8	0	-1.447859	5.547568	-0.162926
19	6	0	-0.639529	6.366694	0.756885
20	8	0	0.064138	3.832384	0.045113
21	6	0	2.292304	-1.261655	0.866397
22	6	0	3.180452	-2.403627	0.868478
23	6	0	2.861539	-3.224010	2.007557
24	6	0	1.767809	-2.606855	2.712578
25	6	0	1.409397	-1.389794	2.019285
26	26	0	1.166933	-3.049885	0.740855
27	6	0	-0.277747	-4.593464	0.855856
28	6	0	0.770928	-4.963818	-0.064732
29	6	0	0.796270	-3.987372	-1.126076
30	6	0	-0.238427	-3.015825	-0.862316
31	6	0	-0.899729	-3.391112	0.361004
32	16	0	0.042167	-0.266007	2.458256
33	6	0	0.637820	0.636318	4.096631
34	6	0	2.014969	1.280565	3.873939
35	6	0	3.253285	-0.573516	-1.812382
36	6	0	2.485811	-1.151702	-2.846990

Anexo VI: Computational methods

37	6	0	3.115230	-1.711060	-3.973773
38	6	0	4.519167	-1.689779	-4.083647
39	6	0	5.287745	-1.101381	-3.061807
40	6	0	4.658332	-0.546891	-1.930208
41	6	0	-0.453761	1.704097	4.319622
42	6	0	0.668566	-0.374700	5.258696
43	1	0	1.269456	-2.991702	3.589882
44	1	0	3.345369	-4.153233	2.274055
45	1	0	3.940076	-2.608019	0.127492
46	1	0	-1.710924	-2.856778	0.832925
47	1	0	-0.495933	-2.168412	-1.481593
48	1	0	-0.545571	-5.116499	1.763404
49	1	0	1.429903	-5.815696	0.031708
50	1	0	1.479762	-3.978566	-1.963302
51	1	0	-4.423688	-0.513626	-2.532946
52	1	0	-4.087069	-2.671708	-3.678081
53	1	0	-0.179251	-1.374795	-4.986309
54	1	0	-0.523952	0.798823	-3.812117
55	1	0	0.907266	0.151550	6.195017
56	1	0	-0.300560	-0.871794	5.380257
57	1	0	1.437128	-1.139850	5.102597
58	1	0	2.328348	1.797102	4.793567
59	1	0	2.776010	0.529613	3.635086
60	1	0	1.987135	2.011927	3.059439
61	1	0	-0.228184	2.264389	5.237660
62	1	0	-0.490813	2.413811	3.484711
63	1	0	-1.445185	1.249047	4.436864
64	1	0	4.777296	-0.156550	1.434801
65	1	0	6.387157	1.479563	2.379188
66	1	0	6.085181	3.925681	1.956922
67	1	0	4.145226	4.717401	0.591460
68	1	0	2.526583	3.084842	-0.344261

69	1	0	1.400993	-1.152344	-2.785596
70	1	0	2.512805	-2.152077	-4.764545
71	1	0	5.005864	-2.115337	-4.957985
72	1	0	6.371510	-1.068182	-3.144220
73	1	0	5.265349	-0.080233	-1.160362
74	1	0	0.351710	6.548200	0.328689
75	1	0	-1.195361	7.299174	0.863809
76	1	0	-0.530501	5.860294	1.721259
77	1	0	-2.067823	4.265520	-2.257552
78	1	0	-2.938603	2.331931	-3.346398
79	1	0	-1.960810	-3.135805	-4.909002
80	47	0	0.197399	1.277452	-0.999239
81	6	0	-3.876902	2.011362	-1.456825
82	6	0	-3.374216	3.337202	-0.785458
83	1	0	-4.037206	4.184216	-0.991790
84	1	0	-3.310343	3.220967	0.301858
85	1	0	-4.776081	2.213683	-2.054699
86	6	0	-4.235503	0.957344	-0.429509
87	6	0	-3.275019	0.432925	0.472693
88	6	0	-5.569767	0.487609	-0.329920
89	6	0	-3.623103	-0.532430	1.423218
90	1	0	-2.250411	0.786207	0.419503
91	6	0	-5.943589	-0.469920	0.621286
92	1	0	-6.323907	0.885445	-1.005763
93	6	0	-4.957972	-0.976238	1.489579
94	1	0	-2.884397	-0.929993	2.110673
95	1	0	-6.964464	-0.826342	0.703035
96	7	0	-5.329809	-1.985923	2.485237
97	8	0	-6.556891	-2.356629	2.552368
98	8	0	-4.411502	-2.462280	3.246508

endo-64a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.985524	0.315966	-0.476806
2	7	0	-2.061642	1.171641	0.276785
3	6	0	-1.092404	1.772608	-0.657068
4	6	0	0.060463	2.476270	0.040232
5	6	0	0.519346	2.066925	1.310798
6	6	0	1.599813	2.726584	1.923955
7	6	0	2.239270	3.800456	1.274832
8	6	0	1.783800	4.217806	0.009173
9	6	0	0.697128	3.562345	-0.598083
10	6	0	-3.528049	-0.832400	0.372520
11	8	0	-4.853826	-1.073039	0.067930
12	6	0	-5.506808	-2.203525	0.757276
13	8	0	-2.896456	-1.506920	1.201166
14	1	0	0.339524	3.900824	-1.569924
15	1	0	2.266174	5.051584	-0.495827
16	1	0	1.944145	2.402160	2.903183
17	1	0	0.025031	1.238702	1.809024
18	1	0	-5.504520	-2.034784	1.838503
19	1	0	-6.523616	-2.223245	0.363537
20	1	0	-4.978272	-3.135834	0.535374
21	1	0	-3.857393	0.856313	-0.877901
22	1	0	3.076183	4.307464	1.749278
23	1	0	-1.576402	2.512131	-1.328346
24	6	0	-0.737065	0.539138	-1.579498
25	6	0	-2.108463	-0.208444	-1.675904
26	1	0	-0.455078	0.924297	-2.566384
27	1	0	-2.610605	0.024578	-2.620147

28	1	0	-1.972030	-1.292698	-1.635114
29	6	0	0.410298	-0.321949	-1.070994
30	6	0	1.661217	-0.261608	-1.727733
31	6	0	0.269533	-1.180394	0.046691
32	6	0	2.751603	-1.029002	-1.295537
33	1	0	1.783894	0.394729	-2.586197
34	6	0	1.347847	-1.956219	0.493585
35	1	0	-0.677835	-1.234853	0.574272
36	6	0	2.577409	-1.871304	-0.184158
37	1	0	3.713599	-0.988043	-1.793863
38	1	0	1.251189	-2.615336	1.349148
39	7	0	3.713333	-2.685319	0.280862
40	8	0	3.540987	-3.445557	1.297205
41	8	0	4.823996	-2.596360	-0.352325
42	1	0	-2.479908	1.803248	0.956342

ET1d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.877471	-0.640900	-1.447747
2	6	0	3.631065	-0.024515	-1.722501
3	6	0	3.315251	1.191745	-1.133349
4	6	0	4.224960	1.864595	-0.246899
5	6	0	5.482640	1.209226	0.001121
6	6	0	5.807976	-0.009924	-0.582071
7	6	0	3.943692	3.140822	0.342525
8	6	0	2.321743	1.864596	2.577279
9	7	0	1.306206	2.380215	1.910994
10	6	0	1.399260	3.739509	1.533910

11	6	0	2.787907	3.930832	0.098529
12	6	0	0.196181	4.319593	0.946858
13	8	0	-0.780454	3.692256	0.437818
14	47	0	-0.399515	1.234509	0.960315
15	15	0	-2.351243	-0.299133	0.405972
16	6	0	-3.099101	-1.384778	1.757346
17	6	0	-2.257236	-1.831608	2.797702
18	6	0	-2.761634	-2.651290	3.823728
19	6	0	-4.119155	-3.025023	3.825907
20	6	0	-4.967693	-2.569436	2.798730
21	6	0	-4.461009	-1.754045	1.768792
22	6	0	2.359791	0.501885	3.125582
23	6	0	1.204011	-0.114797	3.668884
24	6	0	1.287591	-1.385322	4.263865
25	6	0	2.518540	-2.069425	4.312853
26	6	0	3.671612	-1.465982	3.771973
27	6	0	3.596476	-0.187038	3.196937
28	7	0	5.187416	-1.912487	-2.038777
29	8	0	4.293223	-2.491846	-2.782951
30	6	0	-3.825541	0.678039	-0.241830
31	6	0	-4.772788	0.114833	-1.123902
32	6	0	-5.869296	0.876125	-1.567477
33	6	0	-6.026945	2.207744	-1.134943
34	6	0	-5.075702	2.777632	-0.267554
35	6	0	-3.975244	2.018019	0.173989
36	6	0	-1.976443	-1.487743	-0.965708
37	6	0	-2.540698	-2.801393	-1.186027
38	6	0	-2.000446	-3.323113	-2.415445
39	6	0	-1.088901	-2.348637	-2.957902
40	6	0	-1.070411	-1.207630	-2.072556
41	26	0	-0.430859	-2.937851	-1.041913
42	6	0	1.535799	-2.684610	-0.247987

43	6	0	1.544739	-3.708066	-1.261492
44	6	0	0.638471	-4.750435	-0.843796
45	6	0	0.070697	-4.370766	0.429341
46	6	0	0.630740	-3.092287	0.794875
47	16	0	-0.060729	0.295273	-2.267842
48	6	0	-0.860680	1.254974	-3.788970
49	6	0	-0.528169	0.493441	-5.086413
50	8	0	0.258959	5.702264	0.914508
51	6	0	-0.855384	6.415133	0.271728
52	6	0	-2.377445	1.401453	-3.596948
53	6	0	-0.151118	2.624510	-3.747220
54	8	0	6.341504	-2.448697	-1.808880
55	1	0	-0.493257	-2.454924	-3.852418
56	1	0	-2.222550	-4.290414	-2.843809
57	1	0	-3.235751	-3.305907	-0.530100
58	1	0	2.112627	-1.772212	-0.269339
59	1	0	0.431874	-2.543163	1.701719
60	1	0	2.146366	-3.686038	-2.159611
61	1	0	0.416173	-5.655356	-1.393117
62	1	0	-0.648076	-4.939699	1.003231
63	1	0	4.487775	0.272780	2.776737
64	1	0	4.623186	-1.990861	3.798635
65	1	0	0.403491	-1.831056	4.715364
66	1	0	0.264146	0.432787	3.674091
67	1	0	-0.887011	1.071197	-5.951195
68	1	0	0.551599	0.343147	-5.196704
69	1	0	-1.021034	-0.484764	-5.111714
70	1	0	-2.800214	1.941291	-4.457505
71	1	0	-2.871097	0.425158	-3.538616
72	1	0	-2.615704	1.962935	-2.688103
73	1	0	-0.504768	3.238764	-4.587080
74	1	0	-0.371790	3.157815	-2.814756

75	1	0	0.936844	2.518656	-3.843947
76	1	0	-4.646488	-0.903153	-1.483494
77	1	0	-6.592345	0.434197	-2.248953
78	1	0	-6.874327	2.796211	-1.478818
79	1	0	-5.180307	3.810288	0.055821
80	1	0	-3.229524	2.479212	0.817273
81	1	0	-1.213637	-1.533364	2.814296
82	1	0	-2.101369	-2.991189	4.618497
83	1	0	-4.511970	-3.653719	4.621302
84	1	0	-6.020383	-2.842374	2.799090
85	1	0	-5.134592	-1.395968	0.996290
86	1	0	-1.782551	6.252103	0.831185
87	1	0	-0.566893	7.467113	0.297592
88	1	0	-0.988659	6.069359	-0.758249
89	1	0	1.903021	4.402168	2.238782
90	1	0	3.187405	2.495089	2.793914
91	1	0	2.580333	-3.053183	4.771439
92	1	0	2.880532	5.007788	0.234872
93	1	0	2.172099	3.668841	-0.762963
94	1	0	4.714597	3.559434	0.990553
95	1	0	2.349731	1.634914	-1.350473
96	1	0	6.203157	1.697346	0.655882
97	1	0	2.934692	-0.513213	-2.394448
98	1	0	6.759860	-0.494780	-0.392148

ET1d'

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-1.058166	-3.020176	1.530296

2	6	0	-1.190132	-3.709878	0.272167
3	6	0	-2.325834	-4.593547	0.369959
4	6	0	-2.893379	-4.449767	1.689365
5	6	0	-2.110004	-3.473642	2.407456
6	26	0	-2.952234	-2.592263	0.673283
7	6	0	-3.296189	-1.149216	-0.873076
8	6	0	-3.215500	-0.512437	0.434206
9	6	0	-4.269848	-1.066592	1.263191
10	6	0	-4.980256	-2.042300	0.486770
11	6	0	-4.377030	-2.102398	-0.823330
12	15	0	-2.094916	0.893113	0.883890
13	6	0	-3.120935	2.412295	0.441752
14	6	0	-4.486929	2.322803	0.102358
15	6	0	-5.215349	3.486723	-0.209282
16	6	0	-4.585092	4.744996	-0.180203
17	6	0	-3.217897	4.832955	0.147399
18	6	0	-2.482156	3.671930	0.449116
19	16	0	-2.215679	-0.622488	-2.249174
20	6	0	-2.637998	-1.728119	-3.801087
21	6	0	-1.635342	-1.206666	-4.855215
22	47	0	0.180399	1.075917	-0.200224
23	7	0	1.967283	1.379968	-1.490924
24	6	0	2.277926	2.715481	-1.815098
25	6	0	1.488433	3.754143	-1.156014
26	8	0	1.748553	5.004506	-1.691924
27	6	0	1.128074	6.162793	-1.030920
28	6	0	2.599479	0.424912	-2.159326
29	6	0	2.569404	-0.995981	-1.806058
30	6	0	2.357352	-1.443279	-0.476107
31	6	0	2.370227	-2.812993	-0.172014
32	6	0	2.597661	-3.766241	-1.185135
33	6	0	2.829430	-3.334633	-2.507100

34	6	0	2.824070	-1.963890	-2.811163
35	6	0	4.129451	3.073164	-1.178035
36	6	0	4.998213	1.984139	-1.453284
37	6	0	5.464310	1.014477	-0.502206
38	6	0	6.475617	0.069365	-0.890063
39	6	0	7.024865	-0.835971	0.009068
40	6	0	6.574939	-0.842247	1.353295
41	6	0	5.564051	0.056643	1.772015
42	6	0	5.019530	0.958688	0.863423
43	7	0	7.149720	-1.763879	2.299400
44	8	0	6.714758	-1.759367	3.519091
45	8	0	0.727272	3.615044	-0.153890
46	6	0	-2.103008	0.890425	2.766157
47	6	0	-0.995503	0.352240	3.453475
48	6	0	-0.975846	0.323447	4.860545
49	6	0	-2.063194	0.840190	5.590751
50	6	0	-3.165071	1.391861	4.908312
51	6	0	-3.185815	1.417672	3.501495
52	8	0	8.082885	-2.566209	1.901231
53	6	0	-2.369649	-3.215523	-3.499859
54	6	0	-4.084797	-1.463291	-4.264978
55	1	0	-4.698971	-2.753966	-1.619133
56	1	0	-5.814318	-2.640932	0.824859
57	1	0	-4.470079	-0.792977	2.288344
58	1	0	-0.548525	-3.578882	-0.586947
59	1	0	-0.302531	-2.287005	1.770319
60	1	0	-2.692240	-5.247385	-0.409646
61	1	0	-3.760034	-4.973332	2.069065
62	1	0	-2.283815	-3.136953	3.419831
63	1	0	3.017185	-1.634171	-3.830806
64	1	0	3.025548	-4.063461	-3.290120
65	1	0	2.236535	-3.141228	0.855866

66	1	0	2.247317	-0.710529	0.319507
67	1	0	-2.577836	-3.809674	-4.401780
68	1	0	-1.321656	-3.372779	-3.221208
69	1	0	-2.996312	-3.598490	-2.689514
70	1	0	-4.285516	-2.044203	-5.177160
71	1	0	-4.826132	-1.750794	-3.513788
72	1	0	-4.231686	-0.402003	-4.493963
73	1	0	-1.783226	-1.759289	-5.793011
74	1	0	-1.786710	-0.140212	-5.061149
75	1	0	-0.599255	-1.356086	-4.529332
76	1	0	-4.982432	1.357128	0.067563
77	1	0	-6.266911	3.408283	-0.474881
78	1	0	-5.148841	5.643754	-0.419340
79	1	0	-2.721470	5.800359	0.160399
80	1	0	-1.418133	3.751786	0.657822
81	1	0	-0.140775	-0.027215	2.897786
82	1	0	-0.114653	-0.088889	5.380020
83	1	0	-2.046684	0.824592	6.677737
84	1	0	-4.001316	1.805604	5.466603
85	1	0	-4.030213	1.866021	2.984543
86	1	0	1.382513	6.176715	0.033874
87	1	0	1.541587	7.032949	-1.543205
88	1	0	0.039365	6.125445	-1.144673
89	1	0	2.618243	-4.825896	-0.942617
90	1	0	3.923865	3.298832	-0.130380
91	1	0	4.243892	3.972181	-1.782908
92	1	0	5.435068	1.927796	-2.451037
93	1	0	6.830011	0.081925	-1.919291
94	1	0	4.253044	1.649023	1.204981
95	1	0	7.797677	-1.536353	-0.289051
96	1	0	5.240112	0.030099	2.807252
97	1	0	3.145990	0.685366	-3.069662

98 1 0 2.506853 2.928954 -2.861677

ET1d-exo

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	8.043418	-0.274492	0.325203
2	6	0	7.492166	-1.004894	-0.757401
3	6	0	6.387806	-0.497282	-1.430540
4	6	0	5.781667	0.754450	-1.068055
5	6	0	6.380759	1.470888	0.024711
6	6	0	7.486310	0.968774	0.708265
7	6	0	4.604538	1.200906	-1.758920
8	6	0	2.923919	-0.070385	0.049620
9	7	0	2.089199	0.948887	-0.130944
10	6	0	2.645781	2.240081	-0.016419
11	6	0	3.916036	2.427391	-1.538291
12	6	0	1.726962	3.368890	-0.168295
13	8	0	0.530263	3.330694	-0.583553
14	47	0	-0.118760	0.854687	-0.253999
15	15	0	-2.517159	0.868349	0.513616
16	6	0	-2.692247	1.256533	2.352369
17	6	0	-1.608466	0.968537	3.208229
18	6	0	-1.698756	1.230504	4.588027
19	6	0	-2.873480	1.792152	5.123564
20	6	0	-3.951833	2.098435	4.270881
21	6	0	-3.862168	1.832801	2.891554
22	6	0	2.665854	-1.463341	-0.319533
23	6	0	3.525470	-2.468906	0.196945
24	6	0	3.372700	-3.812676	-0.180931

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25	6	0	2.363660	-4.181333	-1.093193
26	6	0	1.508710	-3.190689	-1.621928
27	6	0	1.657465	-1.848562	-1.241689
28	7	0	9.175791	-0.806803	1.044797
29	8	0	9.665298	-1.945775	0.677850
30	6	0	-3.541820	2.210745	-0.316706
31	6	0	-4.937518	2.096411	-0.488557
32	6	0	-5.663564	3.139408	-1.092523
33	6	0	-4.998633	4.301877	-1.529189
34	6	0	-3.604193	4.412988	-1.366329
35	6	0	-2.872028	3.370831	-0.764980
36	6	0	-3.512062	-0.678917	0.293987
37	6	0	-4.586403	-1.151781	1.140677
38	6	0	-5.093712	-2.379285	0.585886
39	6	0	-4.334401	-2.684529	-0.598420
40	6	0	-3.356631	-1.638048	-0.793745
41	26	0	-3.035465	-2.587760	1.065292
42	6	0	-1.174887	-3.621907	1.058258
43	6	0	-2.247455	-4.528510	1.382319
44	6	0	-2.888360	-4.051578	2.585079
45	6	0	-2.212951	-2.846883	3.002274
46	6	0	-1.153924	-2.584870	2.057453
47	16	0	-2.111282	-1.576661	-2.126341
48	6	0	-3.135114	-1.106638	-3.738294
49	6	0	-4.054942	-2.282378	-4.117895
50	8	0	2.351425	4.574079	0.099828
51	6	0	1.583576	5.803697	-0.154333
52	6	0	-3.941061	0.179312	-3.498448
53	6	0	-2.035885	-0.895067	-4.799808
54	8	0	9.658675	-0.131086	2.035524
55	1	0	-4.449851	-3.554715	-1.227552
56	1	0	-5.893369	-2.977320	0.999833

57	1	0	-4.930557	-0.674012	2.046437
58	1	0	-0.506814	-3.693952	0.213070
59	1	0	-0.455756	-1.761564	2.089382
60	1	0	-2.528372	-5.407010	0.818083
61	1	0	-3.733445	-4.510113	3.079884
62	1	0	-2.461580	-2.241787	3.862713
63	1	0	1.019995	-1.092651	-1.692194
64	1	0	0.737529	-3.461199	-2.339524
65	1	0	4.043174	-4.566235	0.224734
66	1	0	4.318705	-2.187647	0.886618
67	1	0	-4.564958	-2.056224	-5.065871
68	1	0	-3.484929	-3.209622	-4.247150
69	1	0	-4.825579	-2.448063	-3.357016
70	1	0	-4.491387	0.440706	-4.414362
71	1	0	-4.672294	0.050396	-2.693473
72	1	0	-3.289878	1.020390	-3.237818
73	1	0	-2.505457	-0.650773	-5.762487
74	1	0	-1.369327	-0.067923	-4.527692
75	1	0	-1.429761	-1.798822	-4.939780
76	1	0	-5.456112	1.195071	-0.171901
77	1	0	-6.738821	3.043210	-1.223404
78	1	0	-5.559593	5.107310	-1.997364
79	1	0	-3.083732	5.302637	-1.712176
80	1	0	-1.792769	3.463623	-0.659305
81	1	0	-0.686947	0.559664	2.800364
82	1	0	-0.854744	1.007094	5.235755
83	1	0	-2.942725	2.000948	6.188346
84	1	0	-4.855617	2.548341	4.674622
85	1	0	-4.691661	2.099422	2.242705
86	1	0	0.719199	5.858581	0.515747
87	1	0	2.282961	6.617121	0.045585
88	1	0	1.239918	5.829739	-1.193963

89	1	0	3.411373	2.383804	0.751417
90	1	0	3.870052	0.110988	0.563281
91	1	0	2.253593	-5.219274	-1.398350
92	1	0	4.460234	3.276383	-1.122592
93	1	0	3.216210	2.721485	-2.321525
94	1	0	4.214532	0.534476	-2.525716
95	1	0	5.957308	-1.061742	-2.255029
96	1	0	5.970360	2.431412	0.325858
97	1	0	7.942342	-1.951476	-1.036382
98	1	0	7.934269	1.508291	1.536323

ET2d

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	4.431035	-1.559538	-1.486253
2	6	0	3.374893	-0.675044	-1.806127
3	6	0	3.362317	0.608351	-1.270262
4	6	0	4.393089	1.066966	-0.379811
5	6	0	5.457776	0.142422	-0.095901
6	6	0	5.486311	-1.137004	-0.635193
7	6	0	4.339478	2.349531	0.262147
8	6	0	2.914575	1.950444	1.982795
9	7	0	1.830348	2.380742	1.284393
10	6	0	2.156778	3.667141	0.697028
11	6	0	3.474778	3.465519	-0.256088
12	6	0	1.025794	4.274609	-0.092497
13	8	0	0.049742	3.669150	-0.585561
14	47	0	0.048101	1.302226	0.673262

15	15	0	-2.164316	0.096627	0.720198
16	6	0	-2.491348	-0.933257	2.264072
17	6	0	-1.392013	-1.372711	3.030080
18	6	0	-1.597287	-2.152686	4.184052
19	6	0	-2.903701	-2.493713	4.582843
20	6	0	-4.005147	-2.042219	3.828806
21	6	0	-3.800619	-1.263305	2.675192
22	6	0	3.060276	0.607354	2.577139
23	6	0	2.544112	-0.571332	1.985435
24	6	0	2.747957	-1.824122	2.589497
25	6	0	3.467511	-1.927983	3.795612
26	6	0	3.996459	-0.764923	4.389682
27	6	0	3.799240	0.484883	3.780702
28	7	0	4.420687	-2.896303	-2.013981
29	8	0	3.385360	-3.292334	-2.692954
30	6	0	-3.632049	1.282433	0.717508
31	6	0	-4.722786	1.152214	-0.165178
32	6	0	-5.789501	2.070964	-0.114938
33	6	0	-5.775002	3.124793	0.817258
34	6	0	-4.682740	3.261948	1.697379
35	6	0	-3.614861	2.349227	1.643209
36	6	0	-2.502099	-1.045037	-0.696634
37	6	0	-3.527947	-2.065890	-0.763024
38	6	0	-3.489198	-2.663911	-2.071632
39	6	0	-2.433184	-2.035824	-2.821368
40	6	0	-1.817845	-1.030051	-1.986458
41	26	0	-1.629951	-2.931045	-1.081609
42	6	0	0.379484	-3.669845	-1.183482
43	6	0	-0.545910	-4.671464	-1.645659
44	6	0	-1.460251	-4.974991	-0.570436
45	6	0	-1.104863	-4.153342	0.559979
46	6	0	0.028615	-3.344512	0.175570

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47	16	0	-0.390623	0.000552	-2.456568
48	6	0	-1.151884	1.372948	-3.642385
49	6	0	-1.775922	0.695145	-4.876009
50	8	0	1.213643	5.624703	-0.271021
51	6	0	0.223202	6.349715	-1.090212
52	6	0	-2.182955	2.216960	-2.874219
53	6	0	0.080177	2.214567	-4.033966
54	8	0	5.429260	-3.670710	-1.787817
55	1	0	-2.123734	-2.279692	-3.826832
56	1	0	-4.126168	-3.464841	-2.419822
57	1	0	-4.197667	-2.341632	0.038404
58	1	0	1.201499	-3.259849	-1.755203
59	1	0	0.527199	-2.619934	0.800865
60	1	0	-0.550276	-5.115484	-2.631307
61	1	0	-2.277351	-5.682322	-0.610656
62	1	0	-1.603547	-4.133950	1.518456
63	1	0	4.215595	1.380029	4.240316
64	1	0	4.562650	-0.834500	5.315640
65	1	0	2.377322	-2.725805	2.108293
66	1	0	2.031025	-0.508089	1.030161
67	1	0	-2.125323	1.468619	-5.575950
68	1	0	-1.046014	0.064692	-5.397090
69	1	0	-2.638984	0.078384	-4.602158
70	1	0	-2.597461	2.983330	-3.547241
71	1	0	-3.018054	1.604436	-2.516608
72	1	0	-1.722408	2.722092	-2.019380
73	1	0	-0.231480	3.004388	-4.731841
74	1	0	0.523783	2.693155	-3.153882
75	1	0	0.844326	1.604971	-4.531674
76	1	0	-4.747045	0.344457	-0.890653
77	1	0	-6.625118	1.961748	-0.802212
78	1	0	-6.599592	3.832581	0.855623

79	1	0	-4.659576	4.076698	2.416964
80	1	0	-2.771012	2.470854	2.319990
81	1	0	-0.379469	-1.097589	2.744967
82	1	0	-0.741696	-2.481670	4.768297
83	1	0	-3.062849	-3.092714	5.476291
84	1	0	-5.017325	-2.288736	4.140472
85	1	0	-4.658186	-0.894149	2.118125
86	1	0	-0.774580	6.245989	-0.652821
87	1	0	0.554766	7.388432	-1.073880
88	1	0	0.217041	5.954830	-2.111001
89	1	0	2.465182	4.403126	1.457836
90	1	0	3.493201	2.715019	2.517137
91	1	0	3.630277	-2.900884	4.253258
92	1	0	4.008699	4.421551	-0.267535
93	1	0	3.127975	3.268410	-1.277080
94	1	0	5.225616	2.640603	0.826888
95	1	0	2.538688	1.266656	-1.524357
96	1	0	6.258414	0.460041	0.569116
97	1	0	2.583179	-1.009706	-2.467476
98	1	0	6.291407	-1.829350	-0.413342

Table VI.3. Total electronic energies^a (E, in a.u.), thermal corrections to Gibbs free energies^b (TCGFE, in a.u.), and number of imaginary frequencies^c (NIMAG) of all stationary points discussed in the main text corresponding to the dipolar cycloaddition of p-nitrofenyl-1,3-butadiene (61c) with azomethine ylide derived from imine 48a and Cu/(R)-DTBM-Segphos as catalytic system.

Structure	E	T□□□□	NIMAG(v)
61c	-591.401275	0.131432	0
INT2c	-4873.526875	1.651688	0

INT3c	-4873.526513	1.657828	0
<i>exo-69c</i>	-1184.13382	0.313994	0
ET1c	-4873.518471	1.650535	1 (-379.2775)
ET1c'	-4873.513782	1.652882	1 (-310.0698)
ET1c''	-4873.506498	1.654719	1 (-362.9121)
ET1c-endo	-4873.519408	1.652944	1 (-381.4601)
ET1c'-endo	-4873.515958	1.653500	1 (-314.1941)
ET2c	-4873.508599	1.652944	1 (-287.2906)

^aComputed at M06L/LANL2DZ//ONIOM(B3LYP/LANL2DZ:PM6) level of theory. ^b Computed at 298.15 K ONIOM(B3LYP/LANL2DZ:PM6) level of theory. ^cIf NIMAG=1, the imaginary frequency ν (in parentheses) is given in cm^{-1} .

Cartesian of all the stationary collected in Table VI.3.

61c

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-0.985741	-1.780439	0.000000
2	7	0	-1.497177	-3.158009	0.000000
3	6	0	-1.897526	-0.709836	0.000000
4	6	0	-1.396687	0.596543	0.000000
5	6	0	-0.000000	0.857178	-0.000000
6	6	0	0.888850	-0.253770	-0.000000
7	6	0	0.406739	-1.564938	0.000000
8	1	0	-2.962429	-0.913360	0.000000
9	1	0	-2.091155	1.433463	0.000000
10	6	0	0.456588	2.251941	-0.000000
11	1	0	1.962259	-0.091459	-0.000000
12	1	0	1.076788	-2.417449	0.000000
13	6	0	1.748657	2.689537	-0.000000

14	1	0	-0.334133	3.003889	-0.000000
15	6	0	2.117650	4.100538	-0.000000
16	1	0	2.573905	1.976616	-0.000000
17	6	0	3.397673	4.552999	-0.000000
18	1	0	1.297520	4.820961	-0.000000
19	1	0	3.626525	5.615202	-0.000000
20	1	0	4.245281	3.869344	-0.000000
21	8	0	-0.649569	-4.119661	0.000000
22	8	0	-2.766874	-3.334048	0.000000

INT2c

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-2.761223	-1.875150	-3.147374
2	6	0	-2.599235	-1.323065	-1.873053
3	6	0	-2.561270	0.111665	-1.832991
4	6	0	-2.652486	0.868579	-3.019533
5	6	0	-2.806160	0.272129	-4.293499
6	6	0	-2.866597	-1.111485	-4.318501
7	1	0	-2.617337	1.954960	-2.964481
8	1	0	-2.887978	0.867008	-5.195184
9	6	0	-2.626660	-2.268287	-0.700220
10	6	0	-1.525675	-2.648665	0.141494
11	6	0	-3.821748	-2.955565	-0.462185
12	6	0	-1.688675	-3.648935	1.124062
13	6	0	-3.966747	-3.945892	0.519973
14	6	0	-2.913886	-4.321990	1.335906
15	1	0	-0.843105	-3.927921	1.749631
16	1	0	-3.017801	-5.093222	2.089133

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17	8	0	-2.840929	-3.248591	-3.467485
18	8	0	-3.027669	-1.949606	-5.439029
19	8	0	-5.264705	-4.488214	0.487335
20	8	0	-5.036212	-2.812349	-1.172454
21	6	0	-3.227779	-3.305998	-4.892331
22	6	0	-6.024635	-3.646381	-0.452894
23	1	0	-6.706809	-2.991331	0.118944
24	1	0	-6.541938	-4.283999	-1.170324
25	1	0	-2.570250	-4.004269	-5.412944
26	1	0	-4.288048	-3.571869	-4.966699
27	15	0	-2.283979	1.029981	-0.200846
28	15	0	0.141520	-1.758063	0.049194
29	29	0	-0.084256	0.551616	0.431856
30	6	0	-2.748867	2.783881	-0.634501
31	6	0	-1.734709	3.738116	-0.699164
32	6	0	-4.071760	3.151134	-0.878464
33	6	0	-2.023176	5.087396	-0.968088
34	1	0	-0.687027	3.458327	-0.536080
35	6	0	-4.422059	4.482496	-1.145705
36	1	0	-4.871688	2.404584	-0.856209
37	6	0	-3.383564	5.441831	-1.108433
38	6	0	-3.727796	0.524894	0.837805
39	6	0	-3.565594	0.412837	2.213550
40	6	0	-4.971217	0.297597	0.244504
41	6	0	-4.663229	0.109966	3.041311
42	1	0	-2.580243	0.554687	2.681922
43	6	0	-6.112742	0.078592	1.024620
44	1	0	-5.065105	0.297873	-0.847203
45	6	0	-5.933412	0.039252	2.430065
46	6	0	1.123665	-2.620231	1.379130
47	6	0	1.959700	-3.692093	1.074800
48	6	0	1.036718	-2.150493	2.690449

49	6	0	2.777241	-4.279262	2.053835
50	1	0	2.013308	-4.095835	0.055725
51	6	0	1.833079	-2.693891	3.709335
52	1	0	0.347500	-1.332808	2.950370
53	6	0	2.756335	-3.701063	3.341590
54	6	0	1.019283	-2.418611	-1.438020
55	6	0	2.221593	-1.798050	-1.773780
56	6	0	0.585909	-3.556160	-2.114558
57	6	0	3.060130	-2.337985	-2.762032
58	1	0	2.548503	-0.886065	-1.257269
59	6	0	1.392424	-4.151446	-3.097271
60	1	0	-0.383704	-4.005639	-1.874340
61	6	0	2.649279	-3.552996	-3.357812
62	7	0	1.537229	1.816584	0.548914
63	6	0	2.278409	2.432712	-0.360034
64	6	0	2.127341	1.808752	1.882302
65	1	0	3.114631	3.050026	-0.025649
66	6	0	2.069569	2.429273	-1.807766
67	6	0	2.920056	3.251668	-2.595893
68	6	0	1.088540	1.645333	-2.468639
69	6	0	2.789983	3.295371	-3.991869
70	1	0	3.684892	3.849410	-2.104594
71	6	0	0.958864	1.691543	-3.864661
72	1	0	0.443537	0.986843	-1.890325
73	6	0	1.805899	2.516572	-4.633995
74	1	0	3.451242	3.928395	-4.577599
75	1	0	0.206328	1.077017	-4.354485
76	1	0	1.705105	2.545090	-5.716257
77	6	0	4.363060	-1.593667	-3.099886
78	6	0	5.498368	-2.193465	-2.247987
79	1	0	5.648241	-3.262248	-2.452025
80	1	0	6.449499	-1.685961	-2.447937

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81	1	0	5.297235	-2.079351	-1.176410
82	6	0	4.686900	-1.686847	-4.600315
83	1	0	4.889430	-2.714943	-4.922350
84	1	0	3.849208	-1.328067	-5.207513
85	1	0	5.566322	-1.087295	-4.855032
86	6	0	4.253516	-0.091899	-2.757452
87	1	0	3.413324	0.383529	-3.273267
88	1	0	4.141772	0.088604	-1.672054
89	1	0	5.162113	0.444056	-3.055945
90	6	0	0.892402	-5.418683	-3.807177
91	6	0	-0.639379	-5.576408	-3.672090
92	1	0	-0.948602	-5.758760	-2.637058
93	1	0	-1.162778	-4.676739	-4.015754
94	1	0	-0.999219	-6.422489	-4.265233
95	6	0	1.211095	-5.366410	-5.310759
96	1	0	2.294600	-5.347279	-5.498666
97	1	0	0.804937	-6.231843	-5.840411
98	1	0	0.801601	-4.461550	-5.771250
99	6	0	1.550489	-6.646268	-3.146071
100	1	0	1.206421	-7.575976	-3.610535
101	1	0	2.645744	-6.621937	-3.243847
102	1	0	1.314352	-6.701282	-2.078823
103	6	0	-7.476193	-0.066427	0.333395
104	6	0	-4.401683	-0.121267	4.537242
105	6	0	-4.554315	1.223686	5.273816
106	1	0	-3.842595	1.966927	4.900113
107	1	0	-5.565175	1.639357	5.151026
108	1	0	-4.376478	1.107928	6.347993
109	6	0	-2.964516	-0.645294	4.759093
110	1	0	-2.798681	-1.587851	4.226270
111	1	0	-2.200666	0.067217	4.419796
112	1	0	-2.773836	-0.831308	5.821256

113	6	0	-5.353535	-1.177442	5.123021
114	1	0	-5.330030	-2.100606	4.532879
115	1	0	-5.083927	-1.431937	6.152310
116	1	0	-6.397235	-0.843155	5.132326
117	6	0	-8.224544	1.275953	0.452818
118	1	0	-9.210813	1.223703	-0.018740
119	1	0	-8.380267	1.564157	1.502253
120	1	0	-7.664004	2.089180	-0.035998
121	6	0	-8.290214	-1.206561	0.967728
122	1	0	-8.490607	-1.020268	2.033982
123	1	0	-9.256918	-1.338188	0.474722
124	1	0	-7.743487	-2.160251	0.914758
125	6	0	-7.330300	-0.386091	-1.172924
126	1	0	-6.939468	0.464341	-1.741477
127	1	0	-6.656287	-1.232650	-1.352897
128	1	0	-8.300260	-0.638377	-1.614034
129	6	0	-5.888866	4.822772	-1.449434
130	6	0	-6.557066	5.301445	-0.145593
131	1	0	-6.502143	4.537941	0.636530
132	1	0	-6.072532	6.209139	0.244717
133	1	0	-7.612709	5.541818	-0.306808
134	6	0	-6.660768	3.583901	-1.961468
135	1	0	-6.155753	3.118857	-2.813656
136	1	0	-6.796072	2.822346	-1.176150
137	1	0	-7.664444	3.865702	-2.299625
138	6	0	-5.993200	5.896479	-2.545199
139	1	0	-7.033488	6.094456	-2.818316
140	1	0	-5.552047	6.852610	-2.230660
141	1	0	-5.459664	5.592048	-3.451800
142	6	0	-0.865017	6.090438	-1.084483
143	6	0	0.446985	5.379122	-1.483942
144	1	0	0.776017	4.657625	-0.729328

145	1	0	0.342620	4.845068	-2.435955
146	1	0	1.260316	6.102410	-1.611573
147	6	0	-1.143372	7.147040	-2.166345
148	1	0	-1.387838	6.678095	-3.125530
149	1	0	-1.992921	7.792969	-1.909616
150	1	0	-0.277835	7.797689	-2.323741
151	6	0	-0.659751	6.755391	0.290963
152	1	0	-1.559442	7.300229	0.613840
153	1	0	-0.426376	6.016872	1.063296
154	1	0	0.162800	7.477908	0.260903
155	8	0	-3.712691	6.789143	-1.309732
156	8	0	3.473293	-4.150429	-4.321076
157	8	0	3.633106	-4.193213	4.317986
158	8	0	-7.067537	-0.174795	3.225873
159	6	0	-7.638146	1.030798	3.793646
160	1	0	-8.027132	1.669164	2.985850
161	1	0	-8.450282	0.635430	4.413713
162	1	0	-6.890981	1.561403	4.403955
163	6	0	4.915534	-3.514032	4.344350
164	1	0	5.442807	-4.039430	5.147480
165	1	0	5.429202	-3.638087	3.378029
166	1	0	4.769832	-2.450536	4.588930
167	6	0	1.678069	-2.168635	5.144317
168	6	0	0.282202	-1.541639	5.357973
169	1	0	0.109110	-0.681118	4.694635
170	1	0	-0.514606	-2.270851	5.183459
171	1	0	0.172471	-1.174634	6.383523
172	6	0	1.824824	-3.307424	6.168094
173	1	0	2.841703	-3.724107	6.174395
174	1	0	1.605685	-2.966158	7.183443
175	1	0	1.148972	-4.137560	5.939079
176	6	0	2.740345	-1.077866	5.386344

177	1	0	2.751537	-0.766803	6.435734
178	1	0	3.750906	-1.434789	5.138262
179	1	0	2.538132	-0.186401	4.782252
180	6	0	3.649163	-5.480138	1.659287
181	6	0	3.019503	-6.251968	0.474488
182	1	0	2.020802	-6.621614	0.728601
183	1	0	2.931782	-5.631134	-0.424955
184	1	0	3.630881	-7.120463	0.208718
185	6	0	3.790042	-6.481422	2.817476
186	1	0	4.333101	-6.052743	3.670367
187	1	0	2.810577	-6.789101	3.198326
188	1	0	4.329365	-7.380957	2.508000
189	6	0	5.028046	-4.948990	1.223584
190	1	0	5.697956	-5.764764	0.936156
191	1	0	4.945265	-4.266185	0.371196
192	1	0	5.519876	-4.393628	2.037630
193	6	0	4.474918	-5.052544	-3.788804
194	1	0	5.024364	-5.347609	-4.689587
195	1	0	5.130022	-4.524901	-3.077749
196	1	0	3.983741	-5.917834	-3.318821
197	6	0	-3.968511	7.528070	-0.088898
198	1	0	-4.184514	8.533748	-0.466699
199	1	0	-4.839121	7.101362	0.431994
200	1	0	-3.071797	7.525967	0.549770
201	1	0	2.636813	2.752406	2.112680
202	6	0	1.087827	1.473576	2.923103
203	8	0	0.069386	0.784534	2.668441
204	8	0	1.300130	1.819158	4.236910
205	6	0	2.339400	2.778020	4.652836
206	1	0	2.137351	3.769534	4.232018
207	1	0	2.257898	2.812849	5.739832
208	1	0	3.338769	2.435301	4.366440

209	6	0	4.355390	0.855511	0.869227
210	6	0	3.332287	0.655206	1.925454
211	1	0	4.213765	0.347638	-0.090066
212	1	0	3.767470	0.716528	2.932038
213	6	0	5.480601	1.666652	1.045281
214	6	0	6.466774	1.952976	0.082616
215	1	0	6.343537	1.502175	-0.903511
216	1	0	2.812994	-0.308411	1.832208
217	1	0	5.597287	2.122118	2.034316
218	6	0	7.618849	2.781421	0.267356
219	6	0	8.518032	3.002910	-0.834159
220	6	0	7.953194	3.433502	1.507538
221	6	0	9.644041	3.808534	-0.721529
222	1	0	8.299039	2.520848	-1.785157
223	6	0	9.076137	4.241498	1.630573
224	1	0	7.317944	3.290718	2.377345
225	6	0	9.930589	4.439114	0.515724
226	1	0	10.314588	3.970245	-1.558725
227	1	0	9.323572	4.729746	2.567271
228	7	0	11.089786	5.278850	0.642752
229	8	0	11.328766	5.846547	1.783337
230	8	0	11.858893	5.443080	-0.386844

INT3c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.560432	-1.357569	-3.574253
2	6	0	-1.843354	-1.087183	-2.233789

3	6	0	-2.140012	0.284268	-1.932818
4	6	0	-2.124902	1.263635	-2.946169
5	6	0	-1.823948	0.954176	-4.295035
6	6	0	-1.539575	-0.372903	-4.573313
7	1	0	-2.350406	2.297459	-2.692028
8	1	0	-1.823916	1.713695	-5.067959
9	6	0	-1.920285	-2.237562	-1.266999
10	6	0	-0.939718	-2.574115	-0.272842
11	6	0	-2.984910	-3.134427	-1.387018
12	6	0	-1.087115	-3.735212	0.513435
13	6	0	-3.117340	-4.286009	-0.596319
14	6	0	-2.183227	-4.618321	0.370220
15	1	0	-0.330720	-3.980993	1.255905
16	1	0	-2.279045	-5.511174	0.976372
17	8	0	-1.289856	-2.620608	-4.144398
18	8	0	-1.246953	-0.949478	-5.825705
19	8	0	-4.259254	-5.016109	-0.976185
20	8	0	-4.051050	-3.067305	-2.312012
21	6	0	-0.915940	-2.360734	-5.551166
22	6	0	-4.972132	-4.165809	-1.947683
23	1	0	-5.872625	-3.743625	-1.465354
24	1	0	-5.197637	-4.750934	-2.840223
25	1	0	0.171103	-2.516013	-5.671235
26	1	0	-1.512455	-3.002243	-6.201671
27	15	0	-2.387784	0.817359	-0.134913
28	15	0	0.533129	-1.416647	0.033512
29	29	0	-0.257665	0.688789	0.853192
30	6	0	-3.133329	2.516274	-0.294069
31	6	0	-2.402379	3.590152	0.204072
32	6	0	-4.390826	2.723211	-0.864273
33	6	0	-2.919743	4.899331	0.162877
34	1	0	-1.400881	3.445379	0.651814

Anexo VI: Computational methods

35	6	0	-4.972916	3.996221	-0.898234
36	1	0	-4.949413	1.882595	-1.286537
37	6	0	-4.234506	5.058364	-0.319583
38	6	0	-3.866439	-0.167093	0.398719
39	6	0	-3.909186	-0.656186	1.698842
40	6	0	-4.924447	-0.386553	-0.483218
41	6	0	-5.045283	-1.342759	2.166434
42	1	0	-3.059912	-0.514203	2.384680
43	6	0	-6.106081	-1.003192	-0.052894
44	1	0	-4.843892	-0.062559	-1.527194
45	6	0	-6.156535	-1.417731	1.299856
46	6	0	1.514505	-2.382690	1.303231
47	6	0	2.629270	-3.139463	0.953271
48	6	0	1.104164	-2.316994	2.635226
49	6	0	3.381840	-3.820694	1.924594
50	1	0	2.954288	-3.216471	-0.091249
51	6	0	1.816515	-2.973927	3.649754
52	1	0	0.209407	-1.738412	2.918726
53	6	0	2.996331	-3.655476	3.272285
54	6	0	1.613402	-1.707688	-1.461283
55	6	0	2.619471	-0.791289	-1.748541
56	6	0	1.463677	-2.864882	-2.225959
57	6	0	3.543082	-1.032819	-2.783147
58	1	0	2.710817	0.135086	-1.169048
59	6	0	2.363433	-3.168549	-3.256212
60	1	0	0.637280	-3.554978	-2.022018
61	6	0	3.426950	-2.257622	-3.476656
62	7	0	0.656392	2.280565	1.699553
63	6	0	1.858588	2.961470	1.212686
64	6	0	1.048192	1.970210	3.077913
65	1	0	2.062925	3.870072	1.820860
66	6	0	1.862367	3.404979	-0.238640

67	6	0	2.603244	4.553191	-0.601905
68	6	0	1.150536	2.730686	-1.253764
69	6	0	2.634499	5.015801	-1.929782
70	1	0	3.153862	5.094991	0.164972
71	6	0	1.168055	3.192881	-2.583051
72	1	0	0.567352	1.847508	-1.001405
73	6	0	1.911450	4.337488	-2.929582
74	1	0	3.211997	5.902865	-2.180802
75	1	0	0.601385	2.658841	-3.344042
76	1	0	1.924213	4.695755	-3.956877
77	6	0	4.610274	0.035640	-3.070089
78	6	0	5.877713	-0.323800	-2.265774
79	1	0	6.389328	-1.200809	-2.688624
80	1	0	6.598590	0.506524	-2.263707
81	1	0	5.636881	-0.555820	-1.223089
82	6	0	4.918636	0.147543	-4.572254
83	1	0	5.333284	-0.775307	-4.992359
84	1	0	4.007107	0.361286	-5.142636
85	1	0	5.634897	0.949107	-4.774957
86	6	0	4.135534	1.433745	-2.619209
87	1	0	3.167254	1.693607	-3.065192
88	1	0	4.029834	1.517423	-1.527639
89	1	0	4.839353	2.214130	-2.928006
90	6	0	2.156311	-4.444310	-4.086804
91	6	0	0.767764	-5.079021	-3.847523
92	1	0	0.670951	-5.487210	-2.835590
93	1	0	-0.049107	-4.359223	-3.984348
94	1	0	0.590886	-5.907244	-4.540904
95	6	0	2.262254	-4.104431	-5.584829
96	1	0	3.260977	-3.717812	-5.839757
97	1	0	2.081398	-4.980406	-6.212545
98	1	0	1.539251	-3.324078	-5.863984

99	6	0	3.206807	-5.497093	-3.682687
100	1	0	3.055409	-6.434251	-4.228303
101	1	0	4.229458	-5.160766	-3.899851
102	1	0	3.151093	-5.723682	-2.613071
103	6	0	-7.268314	-1.151124	-1.044086
104	6	0	-4.999345	-1.951434	3.575088
105	6	0	-5.547084	-0.911314	4.572190
106	1	0	-4.944209	0.002999	4.563459
107	1	0	-6.582281	-0.629447	4.330383
108	1	0	-5.541260	-1.301571	5.594419
109	6	0	-3.544822	-2.298043	3.967663
110	1	0	-3.103541	-3.011553	3.263371
111	1	0	-2.894975	-1.411861	3.989331
112	1	0	-3.502323	-2.747450	4.964405
113	6	0	-5.806224	-3.258723	3.653514
114	1	0	-5.492737	-3.961983	2.873844
115	1	0	-5.677975	-3.750993	4.621313
116	1	0	-6.880517	-3.093263	3.507719
117	6	0	-8.239469	0.025960	-0.823718
118	1	0	-9.116052	-0.054679	-1.473130
119	1	0	-8.599630	0.063799	0.214676
120	1	0	-7.751097	0.989845	-1.041370
121	6	0	-7.988893	-2.497267	-0.856979
122	1	0	-8.452661	-2.577759	0.136960
123	1	0	-8.778232	-2.641961	-1.598701
124	1	0	-7.281049	-3.336218	-0.937299
125	6	0	-6.778008	-1.096288	-2.510267
126	1	0	-6.421691	-0.099593	-2.792041
127	1	0	-5.952000	-1.794775	-2.693706
128	1	0	-7.585798	-1.349512	-3.203974
129	6	0	-6.358733	4.173422	-1.534216
130	6	0	-7.413273	4.211666	-0.409419

131	1	0	-7.378080	3.303204	0.199846
132	1	0	-7.250309	5.066038	0.264151
133	1	0	-8.424110	4.306950	-0.816554
134	6	0	-6.713364	2.996394	-2.474285
135	1	0	-5.936186	2.834554	-3.227370
136	1	0	-6.866454	2.056564	-1.919797
137	1	0	-7.645058	3.198606	-3.013605
138	6	0	-6.412999	5.456779	-2.380466
139	1	0	-7.377410	5.570334	-2.881805
140	1	0	-6.252804	6.356274	-1.768320
141	1	0	-5.630725	5.458552	-3.146441
142	6	0	-2.025866	6.050580	0.649007
143	6	0	-0.534081	5.687724	0.491399
144	1	0	-0.262193	4.784657	1.062427
145	1	0	-0.272550	5.490712	-0.554944
146	1	0	0.111786	6.496246	0.842622
147	6	0	-2.262544	7.334469	-0.165316
148	1	0	-2.162974	7.140829	-1.239045
149	1	0	-3.267075	7.745745	-0.014996
150	1	0	-1.543674	8.113854	0.101874
151	6	0	-2.315597	6.289628	2.145198
152	1	0	-3.370074	6.548472	2.316702
153	1	0	-2.092755	5.394268	2.735689
154	1	0	-1.705672	7.107831	2.538933
155	8	0	-4.815475	6.336347	-0.313859
156	8	0	4.327014	-2.554433	-4.510731
157	8	0	3.773294	-4.258409	4.273957
158	8	0	-7.346702	-1.998183	1.767152
159	6	0	-8.231710	-1.060605	2.430159
160	1	0	-8.556050	-0.288318	1.715907
161	1	0	-9.067484	-1.699400	2.733827
162	1	0	-7.728692	-0.617242	3.303867

163	6	0	4.829772	-3.406986	4.783882
164	1	0	5.306246	-4.046928	5.533969
165	1	0	5.529641	-3.149164	3.974138
166	1	0	4.394543	-2.506930	5.245135
167	6	0	1.288622	-2.913345	5.090948
168	6	0	-0.229347	-2.629304	5.116007
169	1	0	-0.475950	-1.652788	4.667738
170	1	0	-0.792464	-3.397549	4.578209
171	1	0	-0.606635	-2.602688	6.142909
172	6	0	1.511350	-4.250700	5.818684
173	1	0	2.578127	-4.470006	5.958651
174	1	0	1.042972	-4.252312	6.806523
175	1	0	1.093100	-5.085868	5.247433
176	6	0	2.007652	-1.764577	5.826965
177	1	0	1.732421	-1.745562	6.885868
178	1	0	3.100078	-1.866588	5.768619
179	1	0	1.730702	-0.793082	5.399819
180	6	0	4.566711	-4.682764	1.466821
181	6	0	4.365780	-5.171117	0.011920
182	1	0	3.454700	-5.772646	-0.078217
183	1	0	4.290074	-4.339651	-0.698571
184	1	0	5.204609	-5.796898	-0.308210
185	6	0	4.721120	-5.940696	2.338011
186	1	0	4.988040	-5.695373	3.374408
187	1	0	3.783405	-6.504701	2.387720
188	1	0	5.495708	-6.607317	1.949789
189	6	0	5.842598	-3.819387	1.524147
190	1	0	6.723316	-4.390285	1.215290
191	1	0	5.763095	-2.945243	0.870654
192	1	0	6.030197	-3.452569	2.544870
193	6	0	5.570702	-3.166603	-4.089805
194	1	0	6.124071	-3.240111	-5.032777

195	1	0	6.097015	-2.525701	-3.367224
196	1	0	5.367734	-4.163060	-3.670136
197	6	0	-5.488967	6.677854	0.922693
198	1	0	-5.805531	7.710155	0.740421
199	1	0	-6.354475	6.013499	1.067020
200	1	0	-4.788637	6.617557	1.770438
201	1	0	1.086323	2.883254	3.706357
202	6	0	0.105237	0.975010	3.733122
203	8	0	-0.610745	0.179470	3.086190
204	8	0	0.042254	0.886357	5.107918
205	6	0	0.748506	1.822901	5.996884
206	1	0	0.321883	2.828643	5.913146
207	1	0	0.577365	1.428019	7.000000
208	1	0	1.822240	1.845063	5.783235
209	6	0	3.047964	1.928642	1.612065
210	6	0	2.550288	1.412002	2.996840
211	1	0	2.987371	1.121912	0.869640
212	1	0	3.172456	1.788416	3.820673
213	6	0	4.427554	2.501059	1.622851
214	6	0	5.354188	2.266934	0.653743
215	1	0	5.064560	1.597303	-0.164074
216	1	0	2.571202	0.314398	3.032721
217	1	0	4.661194	3.178988	2.448146
218	6	0	6.708054	2.821709	0.557122
219	6	0	7.517341	2.460132	-0.555508
220	6	0	7.265220	3.704670	1.525592
221	6	0	8.817967	2.949317	-0.706502
222	1	0	7.107126	1.783720	-1.309840
223	6	0	8.562473	4.202626	1.391518
224	1	0	6.677089	4.001154	2.388927
225	6	0	9.332608	3.819961	0.273389
226	1	0	9.435949	2.676616	-1.554652

227	1	0	8.992432	4.875189	2.125519
228	7	0	10.693453	4.338083	0.130269
229	8	0	11.143132	5.131025	1.035375
230	8	0	11.380052	3.977105	-0.893424

exo-69c

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	7	0	-3.534813	-0.051409	1.268395
2	6	0	-2.155768	0.490635	1.124273
3	6	0	-3.658062	-1.423040	0.770100
4	1	0	-1.661477	0.497441	2.108570
5	6	0	-2.108647	1.908926	0.568392
6	6	0	-1.343489	2.896615	1.222306
7	6	0	-2.808765	2.254903	-0.611908
8	6	0	-1.264691	4.205209	0.708986
9	1	0	-0.809289	2.642673	2.136454
10	6	0	-2.734602	3.563282	-1.121836
11	1	0	-3.413275	1.507559	-1.121489
12	6	0	-1.961442	4.542611	-0.466274
13	1	0	-0.669481	4.955527	1.224270
14	1	0	-3.279570	3.819208	-2.027707
15	1	0	-1.906799	5.553497	-0.863704
16	1	0	-4.173673	-2.068001	1.493247
17	6	0	-4.409508	-1.505823	-0.580237
18	8	0	-4.566858	-0.535102	-1.332559
19	8	0	-4.907197	-2.735958	-0.983645
20	6	0	-4.904260	-3.924896	-0.118630

21	1	0	-5.574552	-3.784168	0.737327
22	1	0	-5.283677	-4.726977	-0.753794
23	1	0	-3.895154	-4.175430	0.226258
24	6	0	-1.427620	-0.575947	0.224221
25	6	0	-2.174565	-1.884523	0.600665
26	1	0	-1.632302	-0.333325	-0.825806
27	1	0	-1.805877	-2.270271	1.560011
28	6	0	0.055732	-0.647617	0.451990
29	6	0	0.990119	-0.374566	-0.491360
30	1	0	0.641905	-0.086348	-1.484140
31	1	0	-2.043616	-2.665635	-0.155326
32	1	0	0.360744	-0.933485	1.461679
33	6	0	2.454146	-0.416890	-0.326902
34	6	0	3.272262	-0.098031	-1.441827
35	6	0	3.092004	-0.761341	0.895671
36	6	0	4.669232	-0.118644	-1.354638
37	1	0	2.801335	0.169916	-2.384587
38	6	0	4.485060	-0.787459	1.002402
39	1	0	2.496389	-1.008948	1.769038
40	6	0	5.261934	-0.465189	-0.127816
41	1	0	5.297713	0.124809	-2.203912
42	1	0	4.979952	-1.048400	1.931238
43	7	0	6.727697	-0.492000	-0.020528
44	8	0	7.247561	-0.810713	1.106963
45	8	0	7.417702	-0.195994	-1.058992
46	1	0	-4.283569	0.587083	1.017696

ET1c

Center	Atomic	Atomic	Coordinates (Angstroms)
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Number	Number	Type	X	Y	Z
1	6	0	4.159211	2.016395	-1.905393
2	6	0	3.395989	1.228821	-1.038400
3	6	0	3.018125	-0.055189	-1.556515
4	6	0	3.373747	-0.430908	-2.869107
5	6	0	4.128191	0.405234	-3.726350
6	6	0	4.524230	1.623681	-3.199968
7	1	0	3.097196	-1.415543	-3.240308
8	1	0	4.406073	0.092626	-4.725795
9	6	0	3.227413	1.743577	0.367391
10	6	0	2.034631	2.240392	0.999240
11	6	0	4.400861	1.886382	1.115314
12	6	0	2.106535	2.841577	2.275051
13	6	0	4.450303	2.471282	2.388636
14	6	0	3.314486	2.973624	2.998459
15	1	0	1.199530	3.221379	2.740700
16	1	0	3.344538	3.443234	3.973942
17	8	0	4.696015	3.297035	-1.632060
18	8	0	5.313593	2.623883	-3.807654
19	8	0	5.774053	2.508036	2.864002
20	8	0	5.706524	1.522541	0.711855
21	6	0	5.688765	3.524301	-2.699298
22	6	0	6.562612	1.718014	1.900785
23	1	0	6.801018	0.733597	2.343895
24	1	0	7.449012	2.284145	1.613211
25	1	0	5.629938	4.557921	-3.037782
26	1	0	6.682762	3.243949	-2.329087
27	15	0	2.040280	-1.250766	-0.460271
28	15	0	0.308201	1.943153	0.276989
29	29	0	-0.058806	-0.351938	0.042431
30	6	0	2.056923	-2.849655	-1.410501

31	6	0	1.283247	-2.941885	-2.569777
32	6	0	2.763684	-3.957167	-0.949907
33	6	0	1.206749	-4.139792	-3.296271
34	1	0	0.709024	-2.081078	-2.935216
35	6	0	2.694887	-5.192202	-1.616258
36	1	0	3.376793	-3.896707	-0.042407
37	6	0	1.851085	-5.271315	-2.745004
38	6	0	3.229045	-1.587722	0.915429
39	6	0	2.737156	-1.688287	2.211635
40	6	0	4.594469	-1.726997	0.655809
41	6	0	3.596175	-1.978849	3.286975
42	1	0	1.662318	-1.546012	2.428652
43	6	0	5.492717	-2.034639	1.686024
44	1	0	4.977617	-1.602020	-0.362327
45	6	0	4.950463	-2.224888	2.980766
46	6	0	-0.794526	2.712307	1.568272
47	6	0	-1.252111	4.020863	1.431429
48	6	0	-1.173492	1.947845	2.672955
49	6	0	-2.158676	4.574811	2.348684
50	1	0	-0.924603	4.646323	0.591590
51	6	0	-2.051360	2.459948	3.640601
52	1	0	-0.790414	0.922069	2.806238
53	6	0	-2.597018	3.744019	3.403349
54	6	0	0.014976	3.136042	-1.111059
55	6	0	-1.281216	3.109455	-1.635587
56	6	0	0.944275	4.067917	-1.556523
57	6	0	-1.711213	4.081860	-2.547128
58	1	0	-1.998793	2.342193	-1.317826
59	6	0	0.571914	5.054911	-2.489588
60	1	0	1.975524	4.057004	-1.181752
61	6	0	-0.778313	5.086413	-2.900480
62	7	0	-1.821299	-1.393245	-0.262848

Anexo VI: Computational methods

63	6	0	-2.538743	-1.620395	-1.349416
64	6	0	-2.351289	-1.866854	0.973876
65	1	0	-3.410556	-2.276609	-1.275647
66	6	0	-2.279845	-1.075792	-2.684871
67	6	0	-3.134892	-1.481719	-3.744771
68	6	0	-1.249976	-0.142878	-2.977204
69	6	0	-2.972444	-0.972204	-5.042434
70	1	0	-3.934149	-2.191415	-3.539365
71	6	0	-1.089131	0.367547	-4.274105
72	1	0	-0.590208	0.200436	-2.181873
73	6	0	-1.949020	-0.042079	-5.315200
74	1	0	-3.641391	-1.293144	-5.837024
75	1	0	-0.301575	1.093088	-4.472980
76	1	0	-1.825785	0.360371	-6.317727
77	6	0	-3.154728	4.029184	-3.070835
78	6	0	-4.006090	5.001618	-2.230021
79	1	0	-3.718173	6.047751	-2.408700
80	1	0	-5.068661	4.911270	-2.477772
81	1	0	-3.899599	4.810099	-1.150636
82	6	0	-3.215330	4.399257	-4.562461
83	1	0	-2.872136	5.426348	-4.747822
84	1	0	-2.575039	3.741496	-5.159107
85	1	0	-4.234049	4.319702	-4.952628
86	6	0	-3.754511	2.612884	-2.931632
87	1	0	-3.164587	1.867509	-3.479216
88	1	0	-3.822548	2.286176	-1.887876
89	1	0	-4.770928	2.576366	-3.339015
90	6	0	1.631448	6.053310	-2.977393
91	6	0	3.040799	5.427235	-2.917857
92	1	0	3.320209	5.119598	-1.900398
93	1	0	3.104179	4.536581	-3.554860
94	1	0	3.796102	6.139297	-3.262956

95	6	0	1.398447	6.469448	-4.439995
96	1	0	0.492656	7.074890	-4.563765
97	1	0	2.235969	7.055083	-4.829308
98	1	0	1.272823	5.592224	-5.084455
99	6	0	1.598489	7.282442	-2.046919
100	1	0	2.328948	8.035109	-2.359819
101	1	0	0.609334	7.764044	-2.051019
102	1	0	1.828264	7.007473	-1.012673
103	6	0	6.988354	-2.157261	1.363530
104	6	0	3.004000	-2.012594	4.704038
105	6	0	2.587232	-3.463514	5.017299
106	1	0	1.815257	-3.812653	4.323564
107	1	0	3.440468	-4.153158	4.946963
108	1	0	2.179585	-3.546073	6.029935
109	6	0	1.756136	-1.107270	4.794516
110	1	0	2.006033	-0.061733	4.586943
111	1	0	0.967781	-1.401015	4.080914
112	1	0	1.309339	-1.149548	5.792342
113	6	0	4.008756	-1.497031	5.748432
114	1	0	4.395821	-0.510665	5.470067
115	1	0	3.547159	-1.408146	6.736073
116	1	0	4.878946	-2.156178	5.850511
117	6	0	7.323416	-3.645326	1.144273
118	1	0	8.388317	-3.784814	0.932928
119	1	0	7.083540	-4.246752	2.033872
120	1	0	6.761066	-4.062691	0.302437
121	6	0	7.849370	-1.576149	2.499298
122	1	0	7.757621	-2.164920	3.423601
123	1	0	8.908996	-1.551639	2.232701
124	1	0	7.532593	-0.553570	2.753798
125	6	0	7.345946	-1.380608	0.075232
126	1	0	6.900039	-1.834068	-0.816600

127	1	0	6.999332	-0.340281	0.119588
128	1	0	8.428271	-1.363904	-0.086368
129	6	0	3.510997	-6.376671	-1.079157
130	6	0	2.597142	-7.214466	-0.163444
131	1	0	2.231384	-6.626208	0.683772
132	1	0	1.718716	-7.589862	-0.710044
133	1	0	3.126813	-8.084183	0.237556
134	6	0	4.723047	-5.888699	-0.251517
135	1	0	5.393048	-5.269455	-0.858319
136	1	0	4.419479	-5.301301	0.622551
137	1	0	5.308144	-6.737529	0.117493
138	6	0	4.070222	-7.236210	-2.225146
139	1	0	4.731605	-8.023315	-1.852933
140	1	0	3.271416	-7.725219	-2.800136
141	1	0	4.636977	-6.628297	-2.938088
142	6	0	0.431506	-4.156025	-4.622168
143	6	0	0.452015	-2.757574	-5.280047
144	1	0	-0.053856	-2.002885	-4.664985
145	1	0	1.474549	-2.417378	-5.466898
146	1	0	-0.068813	-2.772434	-6.243740
147	6	0	1.057452	-5.130339	-5.634416
148	1	0	2.129742	-4.943308	-5.755074
149	1	0	0.958745	-6.177001	-5.320438
150	1	0	0.587992	-5.041599	-6.618452
151	6	0	-1.028882	-4.543614	-4.322015
152	1	0	-1.091304	-5.524446	-3.827941
153	1	0	-1.510872	-3.808878	-3.666795
154	1	0	-1.620491	-4.600836	-5.241361
155	8	0	1.703576	-6.511454	-3.382520
156	8	0	-1.200301	6.109731	-3.761273
157	8	0	-3.549393	4.243608	4.302470
158	8	0	5.824586	-2.597452	4.013188

159	6	0	5.888186	-4.028624	4.236984
160	1	0	6.299384	-4.524915	3.344830
161	1	0	6.575289	-4.103311	5.086749
162	1	0	4.890641	-4.417129	4.495815
163	6	0	-4.921337	3.966642	3.921081
164	1	0	-5.488964	4.437353	4.730772
165	1	0	-5.145627	4.432035	2.949129
166	1	0	-5.090109	2.878467	3.895358
167	6	0	-2.361706	1.626249	4.893820
168	6	0	-1.254657	0.580957	5.153622
169	1	0	-1.140433	-0.127981	4.319792
170	1	0	-0.283117	1.057163	5.318605
171	1	0	-1.481288	-0.015934	6.042916
172	6	0	-2.433044	2.529900	6.138430
173	1	0	-3.279379	3.229237	6.087105
174	1	0	-2.549269	1.942998	7.053623
175	1	0	-1.528622	3.137411	6.241730
176	6	0	-3.694642	0.880771	4.694274
177	1	0	-3.998969	0.366177	5.611368
178	1	0	-4.508804	1.567866	4.420149
179	1	0	-3.622191	0.123572	3.902267
180	6	0	-2.628742	6.020245	2.131587
181	6	0	-1.579223	6.833033	1.335011
182	1	0	-0.619401	6.862602	1.861745
183	1	0	-1.402915	6.417421	0.336417
184	1	0	-1.909126	7.868304	1.202154
185	6	0	-2.837532	6.755674	3.465369
186	1	0	-3.649677	6.314987	4.058644
187	1	0	-1.939144	6.705667	4.090000
188	1	0	-3.082448	7.809941	3.310406
189	6	0	-3.936419	5.976770	1.317149
190	1	0	-4.314284	6.982992	1.114976

191	1	0	-3.794256	5.468969	0.349827
192	1	0	-4.726251	5.432462	1.857579
193	6	0	-1.667514	7.302296	-3.081617
194	1	0	-1.890204	7.974881	-3.917239
195	1	0	-2.576364	7.069721	-2.505720
196	1	0	-0.873982	7.712402	-2.438598
197	6	0	0.552864	-7.266576	-2.923514
198	1	0	0.596871	-8.164490	-3.549364
199	1	0	0.673864	-7.515511	-1.858174
200	1	0	-0.371676	-6.697015	-3.105924
201	1	0	-3.002620	-2.738972	0.905748
202	6	0	-1.400913	-1.849971	2.087366
203	8	0	-0.391878	-1.079881	2.128632
204	8	0	-1.663394	-2.574965	3.236531
205	6	0	-2.675926	-3.640473	3.264857
206	1	0	-2.442558	-4.419766	2.528697
207	1	0	-2.615050	-4.052965	4.273222
208	1	0	-3.681583	-3.242259	3.088696
209	6	0	-4.797860	-0.561774	0.563237
210	6	0	-3.686720	-0.537628	1.464351
211	1	0	-4.764287	0.069573	-0.324256
212	1	0	-3.885821	-0.846993	2.498528
213	6	0	-5.913054	-1.413457	0.750491
214	6	0	-7.006901	-1.547666	-0.101279
215	1	0	-7.004427	-0.957198	-1.018738
216	1	0	-3.030789	0.335428	1.415632
217	1	0	-5.905200	-2.008349	1.669149
218	6	0	-8.157986	-2.390040	0.111739
219	6	0	-9.191138	-2.434071	-0.881055
220	6	0	-8.345799	-3.206238	1.277430
221	6	0	-10.323907	-3.230132	-0.735073
222	1	0	-9.080464	-1.822303	-1.774159

223	6	0	-9.472493	-4.006821	1.435215
224	1	0	-7.598730	-3.199199	2.065682
225	6	0	-10.466704	-4.023119	0.427503
226	1	0	-11.101870	-3.257829	-1.490360
227	1	0	-9.613217	-4.621357	2.317925
228	7	0	-11.637431	-4.855246	0.591484
229	8	0	-11.743951	-5.571993	1.661466
230	8	0	-12.534896	-4.853824	-0.337359

ET1c'

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-1.543255	1.931391	-3.808304
2	6	0	-1.032035	1.857871	-2.509968
3	6	0	0.323691	1.393768	-2.416880
4	6	0	1.044223	1.048319	-3.579874
5	6	0	0.488282	1.132874	-4.878090
6	6	0	-0.817840	1.586701	-4.955598
7	1	0	2.080205	0.726624	-3.493016
8	1	0	1.060793	0.872965	-5.760462
9	6	0	-1.859222	2.481303	-1.413567
10	6	0	-2.527468	1.865628	-0.298164
11	6	0	-2.078111	3.858418	-1.550626
12	6	0	-3.303301	2.657415	0.580079
13	6	0	-2.861493	4.621452	-0.676643
14	6	0	-3.485759	4.049294	0.417016
15	1	0	-3.796160	2.194843	1.432359
16	1	0	-4.085897	4.628460	1.108045

Anexo VI: Computational methods

17	8	0	-2.842324	2.356245	-4.178215
18	8	0	-1.606273	1.777919	-6.109859
19	8	0	-2.888701	5.969400	-1.077893
20	8	0	-1.553876	4.694250	-2.565202
21	6	0	-2.798410	2.512915	-5.646055
22	6	0	-2.183636	6.017692	-2.371906
23	1	0	-1.402780	6.781198	-2.328931
24	1	0	-2.911814	6.190078	-3.171952
25	1	0	-3.690949	2.062791	-6.082458
26	1	0	-2.683134	3.575783	-5.890387
27	15	0	1.103852	1.140898	-0.714474
28	15	0	-2.342158	0.024431	0.146177
29	29	0	-0.146054	-0.581494	0.460050
30	6	0	2.880045	0.683845	-1.073511
31	6	0	3.158763	-0.539926	-1.685157
32	6	0	3.924365	1.514414	-0.673874
33	6	0	4.479438	-0.959436	-1.907334
34	1	0	2.346461	-1.204703	-2.004532
35	6	0	5.265494	1.133630	-0.841145
36	1	0	3.724635	2.487294	-0.207805
37	6	0	5.514897	-0.140904	-1.397455
38	6	0	1.337725	2.843467	-0.029642
39	6	0	1.394381	2.970581	1.354392
40	6	0	1.548917	3.942982	-0.861428
41	6	0	1.741143	4.195428	1.950313
42	1	0	1.178344	2.111958	2.013411
43	6	0	1.899970	5.188449	-0.321923
44	1	0	1.453191	3.837501	-1.946650
45	6	0	2.055140	5.265642	1.084843
46	6	0	-3.362452	-0.076905	1.700393
47	6	0	-4.755130	-0.142595	1.619943
48	6	0	-2.729713	-0.037964	2.940530

Anexo VI: Computational methods

49	6	0	-5.549210	-0.194159	2.772964
50	1	0	-5.255634	-0.157997	0.643535
51	6	0	-3.475796	-0.074371	4.132047
52	1	0	-1.629666	0.018489	3.017541
53	6	0	-4.876326	-0.222701	4.017519
54	6	0	-3.434920	-0.949798	-0.998088
55	6	0	-3.860028	-2.191582	-0.509006
56	6	0	-3.824961	-0.520141	-2.258236
57	6	0	-4.760406	-2.983450	-1.228513
58	1	0	-3.513201	-2.556608	0.466074
59	6	0	-4.715465	-1.292080	-3.038147
60	1	0	-3.462023	0.427507	-2.675025
61	6	0	-5.238355	-2.462202	-2.457426
62	7	0	1.279709	-2.060582	0.724470
63	6	0	1.652196	-3.035881	-0.089660
64	6	0	2.175729	-1.740586	1.796333
65	1	0	2.691575	-3.384511	-0.073598
66	6	0	0.799683	-3.687572	-1.091946
67	6	0	1.383495	-4.685855	-1.916682
68	6	0	-0.580399	-3.404571	-1.257882
69	6	0	0.620121	-5.365966	-2.878884
70	1	0	2.438432	-4.926858	-1.796046
71	6	0	-1.341682	-4.080777	-2.222355
72	1	0	-1.052968	-2.659798	-0.621252
73	6	0	-0.746708	-5.064377	-3.040214
74	1	0	1.086604	-6.126713	-3.499306
75	1	0	-2.399747	-3.842656	-2.338412
76	1	0	-1.339432	-5.587114	-3.786864
77	6	0	-5.185916	-4.342207	-0.652029
78	6	0	-6.509423	-4.150591	0.113760
79	1	0	-7.324602	-3.852711	-0.562732
80	1	0	-6.819101	-5.077815	0.606078

81	1	0	-6.424250	-3.372469	0.889606
82	6	0	-5.349305	-5.392853	-1.763013
83	1	0	-6.146309	-5.126083	-2.470973
84	1	0	-4.430899	-5.498089	-2.349936
85	1	0	-5.595780	-6.375990	-1.351303
86	6	0	-4.123110	-4.886261	0.329447
87	1	0	-3.146949	-5.000224	-0.157639
88	1	0	-3.990469	-4.239267	1.202957
89	1	0	-4.408538	-5.874975	0.705549
90	6	0	-4.976653	-0.806065	-4.471783
91	6	0	-3.615470	-0.813008	-5.202999
92	1	0	-2.883001	-0.150674	-4.731384
93	1	0	-3.182435	-1.819995	-5.214084
94	1	0	-3.716297	-0.493092	-6.244561
95	6	0	-5.935113	-1.681086	-5.293892
96	1	0	-6.973897	-1.572717	-4.972097
97	1	0	-5.898708	-1.418320	-6.356206
98	1	0	-5.679644	-2.747012	-5.210607
99	6	0	-5.555947	0.622742	-4.408322
100	1	0	-5.823175	0.986148	-5.404579
101	1	0	-6.460835	0.655722	-3.793888
102	1	0	-4.840541	1.334743	-3.974322
103	6	0	2.107949	6.383130	-1.264031
104	6	0	1.777525	4.266116	3.484762
105	6	0	3.215888	3.949585	3.944402
106	1	0	3.509898	2.937800	3.644296
107	1	0	3.943266	4.654720	3.517608
108	1	0	3.302098	4.007699	5.034168
109	6	0	0.828847	3.216474	4.106094
110	1	0	-0.207322	3.382569	3.794473
111	1	0	1.099635	2.185559	3.822364
112	1	0	0.857626	3.258380	5.199189

113	6	0	1.324859	5.641251	4.001939
114	1	0	0.343768	5.910710	3.594945
115	1	0	1.250008	5.653039	5.093144
116	1	0	2.011267	6.444706	3.710892
117	6	0	3.619241	6.583147	-1.492255
118	1	0	3.808219	7.416497	-2.176474
119	1	0	4.145824	6.808463	-0.553611
120	1	0	4.079838	5.688220	-1.922762
121	6	0	1.468378	7.651097	-0.672541
122	1	0	1.951598	7.945735	0.271358
123	1	0	1.545282	8.500454	-1.355549
124	1	0	0.410533	7.491088	-0.440506
125	6	0	1.455415	6.138090	-2.644712
126	1	0	1.969336	5.352894	-3.209731
127	1	0	0.406210	5.835593	-2.545582
128	1	0	1.487943	7.043307	-3.258517
129	6	0	6.375668	2.103409	-0.410465
130	6	0	6.841811	1.705924	1.004658
131	1	0	6.034694	1.802234	1.735030
132	1	0	7.201448	0.664951	1.026504
133	1	0	7.671255	2.338028	1.338549
134	6	0	5.861971	3.562398	-0.367019
135	1	0	5.516304	3.887838	-1.354392
136	1	0	5.032830	3.692508	0.337510
137	1	0	6.660734	4.245003	-0.060013
138	6	0	7.553503	2.074300	-1.398115
139	1	0	8.304303	2.830913	-1.155625
140	1	0	8.062474	1.098914	-1.401380
141	1	0	7.216627	2.248478	-2.425253
142	6	0	4.726915	-2.265106	-2.679470
143	6	0	3.539002	-2.573508	-3.621430
144	1	0	2.593272	-2.691768	-3.080508

145	1	0	3.406116	-1.783180	-4.366285
146	1	0	3.711521	-3.507639	-4.167573
147	6	0	5.977411	-2.162814	-3.569027
148	1	0	5.936730	-1.284768	-4.220430
149	1	0	6.899865	-2.071655	-2.978789
150	1	0	6.092355	-3.049300	-4.200255
151	6	0	4.876993	-3.410868	-1.665296
152	1	0	5.762122	-3.274551	-1.021042
153	1	0	4.009645	-3.493931	-0.994123
154	1	0	5.008202	-4.376704	-2.164956
155	8	0	6.842811	-0.558721	-1.528268
156	8	0	-6.223321	-3.183122	-3.145805
157	8	0	-5.638163	-0.297096	5.191633
158	8	0	2.454295	6.492246	1.636086
159	6	0	3.877989	6.602115	1.884103
160	1	0	4.422004	6.585085	0.927215
161	1	0	3.956384	7.582158	2.367234
162	1	0	4.216399	5.797633	2.555225
163	6	0	-5.917774	-1.645029	5.644292
164	1	0	-6.521907	-1.468459	6.541127
165	1	0	-6.486359	-2.194579	4.879037
166	1	0	-4.975869	-2.157939	5.894330
167	6	0	-2.747102	0.068126	5.478168
168	6	0	-1.349058	0.695860	5.293359
169	1	0	-0.713226	0.123929	4.598771
170	1	0	-1.416244	1.717416	4.904408
171	1	0	-0.810334	0.745118	6.244744
172	6	0	-3.537951	0.992064	6.422588
173	1	0	-4.507836	0.558761	6.702555
174	1	0	-2.986092	1.184436	7.347022
175	1	0	-3.747260	1.957504	5.951305
176	6	0	-2.574506	-1.326211	6.107937

177	1	0	-2.116902	-1.255217	7.100270
178	1	0	-3.534809	-1.845534	6.228462
179	1	0	-1.924093	-1.966877	5.490796
180	6	0	-7.076435	-0.216277	2.612945
181	6	0	-7.503631	0.409433	1.263050
182	1	0	-7.167857	1.448857	1.183080
183	1	0	-7.104622	-0.141530	0.404479
184	1	0	-8.594271	0.413827	1.164463
185	6	0	-7.771923	0.599272	3.715194
186	1	0	-7.617777	0.167953	4.712724
187	1	0	-7.379026	1.620932	3.759407
188	1	0	-8.851236	0.660788	3.550398
189	6	0	-7.541910	-1.684861	2.637344
190	1	0	-8.622074	-1.762943	2.482587
191	1	0	-7.045140	-2.278570	1.852541
192	1	0	-7.314643	-2.162422	3.602364
193	6	0	-7.573791	-2.764311	-2.814190
194	1	0	-8.178463	-3.351877	-3.514178
195	1	0	-7.795133	-3.039078	-1.770728
196	1	0	-7.697535	-1.690794	-2.981158
197	6	0	7.326142	-1.383070	-0.434987
198	1	0	8.340683	-1.641057	-0.765507
199	1	0	7.344824	-0.794377	0.492216
200	1	0	6.711431	-2.292228	-0.335302
201	1	0	3.241009	-1.806719	1.542106
202	6	0	1.784965	-0.518133	2.531676
203	8	0	0.626964	-0.013505	2.494193
204	8	0	2.679633	0.081087	3.405197
205	6	0	4.133397	-0.098646	3.278943
206	1	0	4.467562	0.114090	2.253823
207	1	0	4.562483	0.630012	3.968364
208	1	0	4.439606	-1.106245	3.574430

209	6	0	2.512128	-4.398646	2.314336
210	6	0	2.137694	-3.198998	3.035591
211	1	0	1.713006	-5.081992	2.033048
212	1	0	2.889660	-2.808952	3.729327
213	6	0	3.831083	-4.724747	1.905828
214	6	0	4.088099	-5.901497	1.108635
215	6	0	4.976630	-3.894931	2.199917
216	6	0	5.349769	-6.198065	0.614858
217	1	0	3.255201	-6.567535	0.889593
218	6	0	6.241917	-4.184323	1.708203
219	1	0	4.857611	-3.036260	2.853085
220	6	0	6.436948	-5.323800	0.890327
221	1	0	5.530240	-7.080929	0.010599
222	1	0	7.097538	-3.559125	1.938910
223	7	0	7.735982	-5.589656	0.341971
224	8	0	8.683667	-4.725040	0.544595
225	8	0	7.916333	-6.665913	-0.350802
226	6	0	0.773548	-3.213435	3.639296
227	6	0	0.447103	-2.639580	4.815674
228	1	0	0.006117	-3.730624	3.059475
229	1	0	-0.573500	-2.674742	5.203235
230	1	0	1.179136	-2.109040	5.422295

ET1c''

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.487358	0.735474	-2.559522
2	6	0	2.902638	0.193079	-1.413293
3	6	0	2.036854	-0.926485	-1.632079

4	6	0	1.784284	-1.396439	-2.936900
5	6	0	2.376239	-0.808190	-4.080838
6	6	0	3.230196	0.259478	-3.853465
7	1	0	1.120708	-2.246881	-3.082573
8	1	0	2.181046	-1.180463	-5.079110
9	6	0	3.266691	0.772261	-0.077387
10	6	0	2.425954	1.633448	0.705306
11	6	0	4.553422	0.564101	0.419691
12	6	0	2.909675	2.213042	1.893812
13	6	0	5.019462	1.142040	1.609468
14	6	0	4.221426	1.977810	2.373238
15	1	0	2.272510	2.878826	2.469934
16	1	0	4.583775	2.436953	3.284909
17	8	0	4.410047	1.799749	-2.613100
18	8	0	3.970255	0.990061	-4.801611
19	8	0	6.364031	0.787959	1.832040
20	8	0	5.579469	-0.199122	-0.178424
21	6	0	4.648847	2.064822	-4.047963
22	6	0	6.694097	-0.207319	0.792967
23	1	0	6.764682	-1.207257	1.257987
24	1	0	7.610780	0.095385	0.285257
25	1	0	4.203461	3.038886	-4.315513
26	1	0	5.721215	2.016470	-4.244306
27	15	0	1.109653	-1.703248	-0.178419
28	15	0	0.637228	1.919743	0.123364
29	29	0	-0.507942	-0.174990	0.499666
30	6	0	0.673960	-3.386043	-0.838981
31	6	0	-0.646864	-3.821445	-0.787188
32	6	0	1.670759	-4.218484	-1.350882
33	6	0	-0.993193	-5.121053	-1.202399
34	1	0	-1.446406	-3.170055	-0.414106
35	6	0	1.395464	-5.537176	-1.728219

36	1	0	2.701743	-3.850569	-1.446494
37	6	0	0.061769	-5.984472	-1.566955
38	6	0	2.439340	-2.130982	1.035858
39	6	0	2.273182	-1.781763	2.371573
40	6	0	3.589631	-2.802468	0.619730
41	6	0	3.239657	-2.131441	3.332451
42	1	0	1.382986	-1.224234	2.712941
43	6	0	4.550548	-3.237884	1.540055
44	1	0	3.745174	-3.011234	-0.446938
45	6	0	4.316184	-2.935695	2.903188
46	6	0	0.034301	3.317026	1.202562
47	6	0	-0.266925	4.561780	0.659060
48	6	0	-0.136980	3.088174	2.569800
49	6	0	-0.712115	5.624419	1.464597
50	1	0	-0.171020	4.742585	-0.418504
51	6	0	-0.563537	4.112649	3.427158
52	1	0	0.059861	2.091206	2.992873
53	6	0	-0.900083	5.356408	2.837493
54	6	0	0.943939	2.816892	-1.481208
55	6	0	0.174452	2.536782	-2.606039
56	6	0	1.967735	3.764521	-1.535602
57	6	0	0.379519	3.239898	-3.807159
58	1	0	-0.608312	1.770862	-2.574864
59	6	0	2.205896	4.503644	-2.702978
60	1	0	2.601205	3.950136	-0.660042
61	6	0	1.340138	4.274329	-3.795805
62	7	0	-2.525234	-0.134744	0.884100
63	6	0	-3.570216	-0.067613	0.072753
64	6	0	-2.829501	-0.230398	2.272060
65	6	0	-3.570659	-0.268826	-1.376573
66	6	0	-4.785579	-0.033930	-2.074803
67	6	0	-2.459255	-0.761890	-2.109274

68	6	0	-4.886014	-0.279186	-3.453803
69	1	0	-5.651494	0.331004	-1.526402
70	6	0	-2.566003	-1.021907	-3.482638
71	1	0	-1.523301	-0.964483	-1.591795
72	6	0	-3.777868	-0.778951	-4.165238
73	1	0	-5.824819	-0.089995	-3.968468
74	1	0	-1.708424	-1.416204	-4.026096
75	1	0	-3.855911	-0.981109	-5.230727
76	6	0	-0.434004	2.856969	-5.051612
77	6	0	-1.674470	3.768467	-5.121705
78	1	0	-1.391646	4.829563	-5.180706
79	1	0	-2.281447	3.542231	-6.004441
80	1	0	-2.313793	3.643189	-4.241941
81	6	0	0.409632	2.982565	-6.331755
82	1	0	0.685969	4.023577	-6.544711
83	1	0	1.346432	2.420666	-6.245088
84	1	0	-0.128407	2.603867	-7.205297
85	6	0	-0.903001	1.387961	-4.966751
86	1	0	-0.054634	0.705163	-4.848172
87	1	0	-1.593489	1.225741	-4.129999
88	1	0	-1.436245	1.093654	-5.876776
89	6	0	3.368585	5.505671	-2.722806
90	6	0	4.473203	5.073171	-1.733048
91	1	0	4.141431	5.129696	-0.690408
92	1	0	4.793359	4.038269	-1.916602
93	1	0	5.356374	5.713580	-1.819364
94	6	0	4.016925	5.591150	-4.116507
95	1	0	3.356106	6.071763	-4.849892
96	1	0	4.948638	6.162860	-4.093752
97	1	0	4.237169	4.589051	-4.512902
98	6	0	2.826237	6.884665	-2.302129
99	1	0	3.623042	7.634375	-2.277348

100	1	0	2.056531	7.241574	-3.003006
101	1	0	2.369031	6.851557	-1.302477
102	6	0	5.759984	-4.033154	1.030308
103	6	0	3.056061	-1.619731	4.769084
104	6	0	2.285052	-2.687041	5.570214
105	1	0	1.291734	-2.862357	5.143485
106	1	0	2.819172	-3.648101	5.580234
107	1	0	2.146027	-2.376253	6.610340
108	6	0	2.241832	-0.306614	4.777948
109	1	0	2.751543	0.480517	4.212195
110	1	0	1.239377	-0.429268	4.333998
111	1	0	2.092877	0.057957	5.798243
112	6	0	4.410130	-1.312985	5.431834
113	1	0	5.010272	-0.639948	4.809116
114	1	0	4.279003	-0.838947	6.408342
115	1	0	5.012823	-2.216755	5.582950
116	6	0	5.451755	-5.534751	1.191588
117	1	0	6.293470	-6.150397	0.860498
118	1	0	5.246857	-5.791426	2.241638
119	1	0	4.568921	-5.832689	0.601446
120	6	0	7.038731	-3.661606	1.801286
121	1	0	6.976460	-3.949674	2.860480
122	1	0	7.922186	-4.149402	1.381573
123	1	0	7.206424	-2.574046	1.787792
124	6	0	6.031512	-3.747787	-0.465449
125	1	0	5.252472	-4.174018	-1.118269
126	1	0	6.086267	-2.671109	-0.668827
127	1	0	6.980415	-4.191217	-0.783909
128	6	0	2.535680	-6.419124	-2.255915
129	6	0	3.085361	-7.247679	-1.078212
130	1	0	3.535568	-6.601519	-0.306486
131	1	0	2.290969	-7.836520	-0.596240

132	1	0	3.855668	-7.949061	-1.413006
133	6	0	3.690359	-5.566715	-2.833019
134	1	0	3.335306	-4.890495	-3.617252
135	1	0	4.198665	-4.964752	-2.062857
136	1	0	4.456113	-6.208123	-3.283486
137	6	0	2.046243	-7.337369	-3.388093
138	1	0	2.866949	-7.910823	-3.827346
139	1	0	1.295648	-8.058897	-3.034455
140	1	0	1.570706	-6.761985	-4.189161
141	6	0	-2.477620	-5.517657	-1.224113
142	6	0	-3.366859	-4.283350	-1.485892
143	1	0	-3.374472	-3.575859	-0.636718
144	1	0	-3.054319	-3.734031	-2.379286
145	1	0	-4.412216	-4.578539	-1.635820
146	6	0	-2.777326	-6.525959	-2.347074
147	1	0	-2.425055	-6.156685	-3.315774
148	1	0	-2.287640	-7.493208	-2.182642
149	1	0	-3.851443	-6.717856	-2.432563
150	6	0	-2.836894	-6.113108	0.150451
151	1	0	-2.224609	-6.996441	0.381187
152	1	0	-2.690852	-5.384138	0.955027
153	1	0	-3.888117	-6.420955	0.183593
154	8	0	-0.219828	-7.328220	-1.851110
155	8	0	1.496692	5.063153	-4.945745
156	8	0	-1.331740	6.390173	3.681199
157	8	0	5.245536	-3.394777	3.848899
158	6	0	4.877584	-4.654755	4.465138
159	1	0	4.841191	-5.445163	3.700049
160	1	0	5.698087	-4.819765	5.171414
161	1	0	3.914017	-4.552753	4.988998
162	6	0	-2.768949	6.537191	3.785753
163	1	0	-2.866749	7.430620	4.412454

164	1	0	-3.217392	6.693619	2.792976
165	1	0	-3.195989	5.653846	4.283678
166	6	0	-0.612744	3.860083	4.942181
167	6	0	0.177438	2.593003	5.336151
168	1	0	-0.254752	1.677439	4.903424
169	1	0	1.224245	2.651860	5.023095
170	1	0	0.175411	2.452701	6.422136
171	6	0	0.018901	5.044771	5.695952
172	1	0	-0.542730	5.976501	5.535547
173	1	0	0.050976	4.863693	6.773698
174	1	0	1.042590	5.231130	5.356656
175	6	0	-2.076942	3.660540	5.379760
176	1	0	-2.138083	3.442871	6.450943
177	1	0	-2.681704	4.559982	5.197725
178	1	0	-2.544820	2.827814	4.837907
179	6	0	-0.951501	6.989902	0.802390
180	6	0	-0.139477	7.128569	-0.507999
181	1	0	0.939839	7.010784	-0.332222
182	1	0	-0.435323	6.386722	-1.258599
183	1	0	-0.289759	8.117135	-0.953689
184	6	0	-0.509433	8.143458	1.717721
185	1	0	-1.105101	8.198100	2.637421
186	1	0	0.531885	8.019114	2.034562
187	1	0	-0.596043	9.111303	1.216190
188	6	0	-2.446765	7.106143	0.446710
189	1	0	-2.666149	8.060369	-0.042406
190	1	0	-2.760040	6.304632	-0.230009
191	1	0	-3.082858	7.046297	1.342463
192	6	0	0.679595	6.261802	-4.937781
193	1	0	0.942912	6.732224	-5.891256
194	1	0	-0.386149	5.985884	-4.911916
195	1	0	0.957197	6.899979	-4.085266

196	6	0	-0.203588	-8.181157	-0.677284
197	1	0	-0.471426	-9.158147	-1.093726
198	1	0	0.808280	-8.193741	-0.244770
199	1	0	-0.954796	-7.837855	0.051488
200	6	0	-1.660361	-0.082431	3.151050
201	8	0	-0.463727	-0.152176	2.741084
202	8	0	-1.825692	0.018125	4.521432
203	6	0	-3.113774	0.366139	5.135882
204	1	0	-3.912566	-0.317296	4.833224
205	1	0	-2.941296	0.278287	6.209929
206	1	0	-3.378449	1.406377	4.885929
207	1	0	-3.732749	0.296636	2.593258
208	1	0	-4.547850	0.176279	0.494298
209	6	0	-3.513186	-2.045533	2.519300
210	6	0	-4.408831	-2.381541	1.452067
211	1	0	-3.959479	-1.942031	3.511538
212	1	0	-3.991268	-2.860580	0.560835
213	6	0	-5.796019	-2.085889	1.449098
214	6	0	-6.661287	-2.308744	0.381170
215	1	0	-6.236234	-2.768745	-0.512248
216	1	0	-2.566250	-2.586927	2.545269
217	1	0	-6.195995	-1.620670	2.355366
218	6	0	-8.057820	-1.954419	0.305346
219	6	0	-8.768536	-2.181093	-0.918852
220	6	0	-8.794126	-1.354930	1.380733
221	6	0	-10.103535	-1.820168	-1.076581
222	1	0	-8.237771	-2.641848	-1.749695
223	6	0	-10.129378	-0.989565	1.236204
224	1	0	-8.305525	-1.179458	2.335139
225	6	0	-10.787736	-1.214572	0.003230
226	1	0	-10.632788	-1.988118	-2.008361
227	1	0	-10.683888	-0.532875	2.049038

228	7	0	-12.170102	-0.820525	-0.153590
229	8	0	-12.774448	-0.267092	0.845312
230	8	0	-12.750602	-1.032103	-1.287880

ET1c-endo

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-2.085426	-2.243342	-3.454204
2	6	0	-2.044550	-1.676125	-2.177311
3	6	0	-2.297720	-0.264620	-2.129949
4	6	0	-2.508398	0.466844	-3.317802
5	6	0	-2.512595	-0.138903	-4.596874
6	6	0	-2.318977	-1.510341	-4.625497
7	1	0	-2.715225	1.533603	-3.263009
8	1	0	-2.690829	0.435519	-5.498019
9	6	0	-1.923140	-2.624061	-1.013854
10	6	0	-0.812796	-2.796455	-0.115817
11	6	0	-2.967103	-3.541378	-0.854427
12	6	0	-0.823278	-3.846854	0.828121
13	6	0	-2.966044	-4.568847	0.098970
14	6	0	-1.897256	-4.757904	0.956999
15	1	0	0.023476	-3.973097	1.499434
16	1	0	-1.878899	-5.558289	1.686378
17	8	0	-1.922822	-3.611135	-3.778032
18	8	0	-2.324775	-2.370548	-5.744672
19	8	0	-4.133785	-5.345879	-0.010141
20	8	0	-4.147991	-3.615152	-1.628400
21	6	0	-2.400573	-3.727818	-5.169026

Anexo VI: Computational methods

22	6	0	-4.991268	-4.642849	-0.982308
23	1	0	-5.821969	-4.148055	-0.446666
24	1	0	-5.331557	-5.351796	-1.738018
25	1	0	-1.742595	-4.393790	-5.725776
26	1	0	-3.447179	-4.056903	-5.161443
27	15	0	-2.365092	0.605135	-0.449448
28	15	0	0.608426	-1.545821	0.001767
29	29	0	-0.244847	0.532684	0.608615
30	6	0	-3.012650	2.302653	-0.857734
31	6	0	-2.159397	3.193528	-1.512949
32	6	0	-4.285987	2.709165	-0.469480
33	6	0	-2.562302	4.506865	-1.798186
34	1	0	-1.148642	2.889253	-1.812862
35	6	0	-4.731390	4.021810	-0.700055
36	1	0	-4.966002	2.017443	0.042392
37	6	0	-3.821037	4.917216	-1.301656
38	6	0	-3.824813	-0.202988	0.352227
39	6	0	-3.755903	-0.497093	1.709051
40	6	0	-4.961518	-0.527065	-0.391756
41	6	0	-4.847974	-1.078306	2.377892
42	1	0	-2.844229	-0.280598	2.296155
43	6	0	-6.083284	-1.097234	0.224863
44	1	0	-4.988989	-0.334389	-1.469252
45	6	0	-6.021903	-1.291671	1.626552
46	6	0	1.653045	-2.269391	1.360812
47	6	0	2.708063	-3.135993	1.079112
48	6	0	1.376421	-1.902862	2.676696
49	6	0	3.557276	-3.599312	2.094922
50	1	0	2.907590	-3.459034	0.049809
51	6	0	2.174947	-2.358886	3.737816
52	1	0	0.526973	-1.239361	2.916208
53	6	0	3.306638	-3.137907	3.407658

54	6	0	1.765632	-1.800264	-1.422636
55	6	0	2.946333	-1.053893	-1.354088
56	6	0	1.566687	-2.724725	-2.441250
57	6	0	4.001145	-1.285272	-2.246414
58	1	0	3.081285	-0.289401	-0.578749
59	6	0	2.584217	-2.978815	-3.380863
60	1	0	0.622100	-3.276559	-2.522913
61	6	0	3.813877	-2.305975	-3.209102
62	7	0	0.451624	2.350609	1.327633
63	6	0	1.124659	3.315074	0.726191
64	6	0	0.063205	2.573897	2.681772
65	1	0	1.292342	4.250547	1.265356
66	6	0	1.682323	3.272112	-0.627479
67	6	0	2.484109	4.367558	-1.045121
68	6	0	1.471226	2.208948	-1.544453
69	6	0	3.055155	4.399126	-2.327036
70	1	0	2.674795	5.181886	-0.349402
71	6	0	2.035892	2.244197	-2.827849
72	1	0	0.868783	1.350448	-1.250692
73	6	0	2.831449	3.339406	-3.227693
74	1	0	3.678465	5.239672	-2.620533
75	1	0	1.865828	1.415910	-3.514611
76	1	0	3.274869	3.360054	-4.220170
77	6	0	5.291408	-0.461090	-2.109744
78	6	0	6.309640	-1.290534	-1.301964
79	1	0	6.650521	-2.171512	-1.865279
80	1	0	7.201764	-0.697935	-1.068664
81	1	0	5.887185	-1.648735	-0.351260
82	6	0	5.861612	-0.089039	-3.488296
83	1	0	6.142715	-0.973812	-4.074950
84	1	0	5.130484	0.466110	-4.084051
85	1	0	6.757528	0.533808	-3.392913

86	6	0	5.035542	0.861076	-1.356066
87	1	0	4.288020	1.481357	-1.864490
88	1	0	4.696465	0.701916	-0.327649
89	1	0	5.951037	1.463637	-1.298742
90	6	0	2.323167	-3.984839	-4.511052
91	6	0	0.817276	-4.063557	-4.838529
92	1	0	0.217216	-4.379784	-3.973869
93	1	0	0.432134	-3.089200	-5.163309
94	1	0	0.633389	-4.780116	-5.644393
95	6	0	3.033965	-3.579159	-5.813817
96	1	0	4.125555	-3.653888	-5.735278
97	1	0	2.725229	-4.208076	-6.653351
98	1	0	2.815394	-2.537628	-6.074855
99	6	0	2.796263	-5.374378	-4.038596
100	1	0	2.644750	-6.129185	-4.816565
101	1	0	3.868074	-5.371444	-3.789925
102	1	0	2.250783	-5.701131	-3.147847
103	6	0	-7.300682	-1.469094	-0.632720
104	6	0	-4.688391	-1.428713	3.865166
105	6	0	-5.182452	-0.227461	4.696525
106	1	0	-4.571792	0.661665	4.505530
107	1	0	-6.227272	0.022297	4.464012
108	1	0	-5.124277	-0.440903	5.768502
109	6	0	-3.205906	-1.692045	4.209310
110	1	0	-2.807444	-2.538109	3.640247
111	1	0	-2.561935	-0.822068	3.993954
112	1	0	-3.081776	-1.919607	5.272046
113	6	0	-5.468381	-2.702796	4.231396
114	1	0	-5.201563	-3.532572	3.567581
115	1	0	-5.260474	-3.016675	5.258276
116	1	0	-6.552721	-2.567598	4.141653
117	6	0	-8.319986	-0.315169	-0.567233

118	1	0	-9.220208	-0.548599	-1.144508
119	1	0	-8.635485	-0.116349	0.467896
120	1	0	-7.900404	0.612827	-0.968903
121	6	0	-7.944048	-2.779162	-0.143722
122	1	0	-8.386454	-2.668393	0.856898
123	1	0	-8.737482	-3.116330	-0.815447
124	1	0	-7.195759	-3.581834	-0.061648
125	6	0	-6.895697	-1.682531	-2.109552
126	1	0	-6.574864	-0.750956	-2.588064
127	1	0	-6.068565	-2.398059	-2.202724
128	1	0	-7.735626	-2.066732	-2.696562
129	6	0	-6.154849	4.411304	-0.276613
130	6	0	-6.082503	5.049748	1.124810
131	1	0	-5.677895	4.350071	1.862209
132	1	0	-5.438937	5.942444	1.124050
133	1	0	-7.073152	5.362637	1.469114
134	6	0	-7.073892	3.169447	-0.205012
135	1	0	-7.140599	2.671379	-1.178741
136	1	0	-6.721905	2.433527	0.526947
137	1	0	-8.090310	3.454083	0.086109
138	6	0	-6.794139	5.381004	-1.284494
139	1	0	-7.841574	5.581090	-1.043112
140	1	0	-6.273886	6.348463	-1.312303
141	1	0	-6.753375	4.979352	-2.302574
142	6	0	-1.623831	5.411517	-2.611152
143	6	0	-0.723546	4.568527	-3.542365
144	1	0	-0.047898	3.908893	-2.983227
145	1	0	-1.316121	3.952370	-4.224600
146	1	0	-0.085454	5.213645	-4.156714
147	6	0	-2.410216	6.378944	-3.512034
148	1	0	-3.137616	5.842696	-4.130619
149	1	0	-2.978821	7.117624	-2.933519

150	1	0	-1.744833	6.932894	-4.180777
151	6	0	-0.729096	6.187250	-1.625563
152	1	0	-1.326942	6.792882	-0.929229
153	1	0	-0.108279	5.507257	-1.030700
154	1	0	-0.053563	6.866504	-2.155877
155	8	0	-4.214223	6.252386	-1.474936
156	8	0	4.868850	-2.596812	-4.084576
157	8	0	4.176131	-3.533424	4.433483
158	8	0	-7.161647	-1.793546	2.273775
159	6	0	-8.020261	-0.762783	2.823687
160	1	0	-8.424766	-0.144089	2.008254
161	1	0	-8.809050	-1.347691	3.308839
162	1	0	-7.464443	-0.157724	3.557130
163	6	0	5.262318	-2.602252	4.674599
164	1	0	5.807169	-3.084812	5.493045
165	1	0	5.888962	-2.514942	3.773706
166	1	0	4.859503	-1.625232	4.984118
167	6	0	1.789212	-1.959205	5.169935
168	6	0	0.273812	-1.675418	5.273618
169	1	0	-0.053351	-0.872689	4.594772
170	1	0	-0.317333	-2.564801	5.032868
171	1	0	0.000304	-1.364499	6.286465
172	6	0	2.104027	-3.080202	6.174620
173	1	0	3.181239	-3.276320	6.252745
174	1	0	1.743650	-2.831268	7.176646
175	1	0	1.637845	-4.024160	5.873664
176	6	0	2.560213	-0.673290	5.525725
177	1	0	2.290819	-0.309275	6.521624
178	1	0	3.647837	-0.840202	5.521351
179	1	0	2.349610	0.129710	4.806514
180	6	0	4.713858	-4.535650	1.716954
181	6	0	4.404349	-5.305316	0.410427

182	1	0	3.497935	-5.911242	0.512759
183	1	0	4.267065	-4.633556	-0.444398
184	1	0	5.223636	-5.986326	0.157949
185	6	0	4.965547	-5.592165	2.805105
186	1	0	5.299648	-5.141278	3.749319
187	1	0	4.051391	-6.149213	3.035874
188	1	0	5.730715	-6.310836	2.499129
189	6	0	5.968586	-3.669902	1.490783
190	1	0	6.825428	-4.279740	1.189679
191	1	0	5.803545	-2.912913	0.707564
192	1	0	6.256144	-3.133378	2.407816
193	6	0	5.736835	-3.669982	-3.640876
194	1	0	6.447186	-3.752247	-4.471240
195	1	0	6.247934	-3.376803	-2.710758
196	1	0	5.160816	-4.598641	-3.512530
197	6	0	-3.801998	7.124943	-0.392233
198	1	0	-4.171858	8.101152	-0.724196
199	1	0	-4.288140	6.810451	0.543690
200	1	0	-2.704517	7.123659	-0.301919
201	1	0	-0.169483	3.608526	2.938369
202	6	0	-0.832738	1.553722	3.224746
203	8	0	-0.915833	0.375789	2.757279
204	8	0	-1.533657	1.797301	4.396139
205	6	0	-1.726464	3.159251	4.911631
206	1	0	-2.238895	3.787227	4.171516
207	1	0	-2.358000	3.034412	5.792818
208	1	0	-0.775313	3.618987	5.203181
209	6	0	2.651596	3.398613	3.510263
210	6	0	1.672540	2.405065	3.808265
211	1	0	2.514808	4.393273	3.942360
212	1	0	1.160363	2.499405	4.768333
213	6	0	3.806751	3.187616	2.718928

214	6	0	4.780907	4.149395	2.453968
215	1	0	4.602732	5.157496	2.833076
216	1	0	1.932505	1.365639	3.575977
217	1	0	3.942698	2.178386	2.321802
218	6	0	6.019509	3.949706	1.747633
219	6	0	6.881174	5.070538	1.504931
220	6	0	6.470564	2.672668	1.271804
221	6	0	8.089509	4.941865	0.827067
222	1	0	6.572126	6.050806	1.863291
223	6	0	7.676935	2.530446	0.594781
224	1	0	5.863901	1.789174	1.450669
225	6	0	8.490861	3.666102	0.363920
226	1	0	8.733981	5.795055	0.644228
227	1	0	8.017259	1.563585	0.239670
228	7	0	9.740037	3.518783	-0.344296
229	8	0	10.084441	2.342408	-0.757860
230	8	0	10.470117	4.566210	-0.543263

ET1c'-endo

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.802831	-3.051286	-3.269858
2	6	0	-1.040560	-2.392185	-2.060666
3	6	0	-1.779995	-1.166331	-2.173608
4	6	0	-2.200337	-0.694955	-3.435330
5	6	0	-1.930944	-1.388038	-4.638813
6	6	0	-1.230501	-2.576699	-4.516390
7	1	0	-2.778737	0.224626	-3.497764

8	1	0	-2.269617	-1.016470	-5.598604
9	6	0	-0.695048	-3.132397	-0.793489
10	6	0	0.289073	-2.824506	0.209932
11	6	0	-1.377878	-4.340855	-0.603733
12	6	0	0.472559	-3.698170	1.306521
13	6	0	-1.168014	-5.200769	0.481005
14	6	0	-0.251822	-4.900254	1.472776
15	1	0	1.206909	-3.455856	2.071587
16	1	0	-0.088230	-5.549200	2.324342
17	8	0	-0.107033	-4.271288	-3.440228
18	8	0	-0.841781	-3.465719	-5.539409
19	8	0	-2.006995	-6.327726	0.392223
20	8	0	-2.381745	-4.881067	-1.444086
21	6	0	-0.349390	-4.669446	-4.841567
22	6	0	-2.640611	-6.244039	-0.935755
23	1	0	-3.717716	-6.388185	-0.830651
24	1	0	-2.169933	-6.972878	-1.605528
25	1	0	0.591460	-4.987814	-5.292774
26	1	0	-1.127298	-5.441850	-4.866222
27	15	0	-2.101512	-0.129065	-0.629040
28	15	0	1.336236	-1.235720	0.196110
29	29	0	0.058695	0.680975	0.184172
30	6	0	-3.235507	1.237619	-1.223812
31	6	0	-2.702716	2.254819	-2.017657
32	6	0	-4.567586	1.291604	-0.823066
33	6	0	-3.482163	3.354534	-2.408604
34	1	0	-1.656473	2.219255	-2.347813
35	6	0	-5.390416	2.377283	-1.166567
36	1	0	-5.008310	0.489392	-0.216529
37	6	0	-4.798515	3.429134	-1.897539
38	6	0	-3.295717	-1.117499	0.380469
39	6	0	-3.335888	-0.859642	1.746049

Anexo VI: Computational methods

40	6	0	-4.189242	-2.014559	-0.207137
41	6	0	-4.329649	-1.433999	2.558410
42	1	0	-2.597457	-0.190503	2.223362
43	6	0	-5.207095	-2.606890	0.552349
44	1	0	-4.106746	-2.253560	-1.271912
45	6	0	-5.294204	-2.240610	1.919493
46	6	0	2.284042	-1.398544	1.786384
47	6	0	3.411382	-2.220848	1.863518
48	6	0	1.846414	-0.699604	2.907827
49	6	0	4.149143	-2.328606	3.048730
50	1	0	3.745184	-2.790114	0.987278
51	6	0	2.547029	-0.770717	4.125359
52	1	0	0.943508	-0.064813	2.874074
53	6	0	3.736379	-1.529514	4.142848
54	6	0	2.708727	-1.488449	-1.025942
55	6	0	3.864139	-0.727858	-0.808755
56	6	0	2.635184	-2.360853	-2.103409
57	6	0	5.001890	-0.892856	-1.606386
58	1	0	3.910871	0.001907	0.010865
59	6	0	3.747310	-2.550618	-2.953094
60	1	0	1.721315	-2.927659	-2.316392
61	6	0	4.939559	-1.878824	-2.622151
62	7	0	-0.086635	2.738662	0.120176
63	6	0	0.273854	3.605100	-0.816009
64	6	0	-0.879748	3.265517	1.188718
65	1	0	-0.229247	4.579845	-0.858074
66	6	0	1.239719	3.359917	-1.887680
67	6	0	1.410011	4.357874	-2.882596
68	6	0	2.046044	2.195969	-1.961732
69	6	0	2.335000	4.189651	-3.924198
70	1	0	0.817170	5.269857	-2.829610
71	6	0	2.968834	2.025809	-3.003315

Anexo VI: Computational methods

72	1	0	1.961788	1.435868	-1.188399
73	6	0	3.116643	3.019331	-3.992844
74	1	0	2.455589	4.967969	-4.673215
75	1	0	3.582553	1.125194	-3.038487
76	1	0	3.839610	2.889773	-4.794264
77	6	0	6.235070	-0.014172	-1.335907
78	6	0	7.193981	-0.791042	-0.412588
79	1	0	7.592259	-1.690222	-0.902869
80	1	0	8.050375	-0.166092	-0.132027
81	1	0	6.698230	-1.107062	0.519038
82	6	0	6.939861	0.374872	-2.645843
83	1	0	7.354040	-0.493580	-3.172334
84	1	0	6.250859	0.870187	-3.337077
85	1	0	7.766786	1.069178	-2.455742
86	6	0	5.830993	1.294699	-0.631402
87	1	0	5.123611	1.883016	-1.226441
88	1	0	5.391140	1.124075	0.355849
89	1	0	6.707356	1.948789	-0.469467
90	6	0	3.525514	-3.420137	-4.199273
91	6	0	2.454933	-2.706423	-5.055956
92	1	0	1.503952	-2.593169	-4.526941
93	1	0	2.790414	-1.701489	-5.338467
94	1	0	2.251562	-3.251201	-5.982289
95	6	0	4.761455	-3.615506	-5.090487
96	1	0	5.504900	-4.269269	-4.627175
97	1	0	4.491209	-4.062613	-6.052123
98	1	0	5.261048	-2.658586	-5.301057
99	6	0	3.030913	-4.811552	-3.750296
100	1	0	2.923212	-5.488079	-4.602249
101	1	0	3.736771	-5.272758	-3.052356
102	1	0	2.059138	-4.755504	-3.241369
103	6	0	-6.169032	-3.599497	-0.116184

104	6	0	-4.300619	-1.115056	4.061006
105	6	0	-5.162906	0.142962	4.295785
106	1	0	-4.741590	1.006536	3.767365
107	1	0	-6.194757	-0.002304	3.946949
108	1	0	-5.205748	0.397333	5.359432
109	6	0	-2.858884	-0.810797	4.525852
110	1	0	-2.198366	-1.668481	4.362994
111	1	0	-2.420483	0.049356	3.991878
112	1	0	-2.830843	-0.567826	5.592159
113	6	0	-4.805477	-2.294392	4.907692
114	1	0	-4.267079	-3.215778	4.657694
115	1	0	-4.668277	-2.106218	5.976533
116	1	0	-5.868167	-2.504287	4.744840
117	6	0	-7.495523	-2.879076	-0.430237
118	1	0	-8.204369	-3.555297	-0.918700
119	1	0	-7.980282	-2.505790	0.483124
120	1	0	-7.337760	-2.024820	-1.095704
121	6	0	-6.407193	-4.811852	0.800519
122	1	0	-6.902544	-4.518632	1.738671
123	1	0	-7.037603	-5.564930	0.321884
124	1	0	-5.461936	-5.286004	1.084549
125	6	0	-5.599147	-4.132679	-1.450894
126	1	0	-5.559734	-3.356701	-2.222468
127	1	0	-4.580642	-4.520335	-1.325444
128	1	0	-6.219825	-4.942627	-1.845484
129	6	0	-6.861215	2.360098	-0.725535
130	6	0	-6.972968	3.120459	0.611858
131	1	0	-6.398550	2.626387	1.400732
132	1	0	-6.606330	4.153156	0.516168
133	1	0	-8.014193	3.176633	0.946597
134	6	0	-7.360025	0.911810	-0.511932
135	1	0	-7.291981	0.331268	-1.438865

136	1	0	-6.786061	0.380193	0.256618
137	1	0	-8.408690	0.902698	-0.198101
138	6	0	-7.774337	2.993624	-1.787843
139	1	0	-8.831093	2.884533	-1.528681
140	1	0	-7.577409	4.066374	-1.916677
141	1	0	-7.619607	2.532321	-2.769438
142	6	0	-2.871624	4.403932	-3.349588
143	6	0	-1.753808	3.779584	-4.214003
144	1	0	-0.929800	3.376593	-3.612000
145	1	0	-2.138630	2.968003	-4.839799
146	1	0	-1.314995	4.525337	-4.886207
147	6	0	-3.922417	4.965710	-4.322532
148	1	0	-4.442503	4.161170	-4.853367
149	1	0	-4.696529	5.549019	-3.807492
150	1	0	-3.466023	5.620321	-5.070861
151	6	0	-2.270713	5.533734	-2.490753
152	1	0	-3.039164	6.021039	-1.872896
153	1	0	-1.488258	5.159711	-1.814668
154	1	0	-1.819932	6.309622	-3.118622
155	8	0	-5.574283	4.560138	-2.191487
156	8	0	6.093102	-2.141328	-3.372307
157	8	0	4.503287	-1.561996	5.315080
158	8	0	-6.346122	-2.778585	2.676403
159	6	0	-7.490257	-1.899234	2.811849
160	1	0	-7.969773	-1.768807	1.829754
161	1	0	-8.136687	-2.459149	3.496526
162	1	0	-7.188474	-0.934082	3.246985
163	6	0	5.507411	-0.516859	5.388632
164	1	0	5.957049	-0.693153	6.371541
165	1	0	6.243811	-0.651527	4.581436
166	1	0	5.028642	0.473826	5.338923
167	6	0	1.990049	-0.010193	5.339051

168	6	0	0.459247	0.161252	5.224972
169	1	0	0.160357	0.691639	4.306228
170	1	0	-0.051005	-0.807370	5.219840
171	1	0	0.063682	0.736779	6.066888
172	6	0	2.255720	-0.768429	6.651232
173	1	0	3.324612	-0.818625	6.892903
174	1	0	1.752376	-0.291196	7.496808
175	1	0	1.902133	-1.802950	6.589307
176	6	0	2.644669	1.384124	5.371292
177	1	0	2.299397	1.966078	6.231481
178	1	0	3.740703	1.315384	5.440970
179	1	0	2.409614	1.959035	4.468793
180	6	0	5.353893	-3.279433	3.092960
181	6	0	5.228615	-4.387998	2.020402
182	1	0	4.320374	-4.981752	2.165336
183	1	0	5.209475	-3.980492	1.003779
184	1	0	6.078263	-5.076911	2.074097
185	6	0	5.455436	-3.986729	4.454940
186	1	0	5.650207	-3.277604	5.271970
187	1	0	4.522698	-4.501604	4.706530
188	1	0	6.261984	-4.724810	4.465748
189	6	0	6.625441	-2.460829	2.804379
190	1	0	7.516644	-3.094970	2.797022
191	1	0	6.566801	-1.952611	1.826915
192	1	0	6.784728	-1.682168	3.565702
193	6	0	6.917824	-3.193476	-2.805528
194	1	0	7.700829	-3.308378	-3.563325
195	1	0	7.342136	-2.851325	-1.847582
196	1	0	6.338775	-4.112321	-2.682458
197	6	0	-5.457531	5.620281	-1.209880
198	1	0	-6.120922	6.391238	-1.618361
199	1	0	-5.814878	5.266699	-0.231338

200	1	0	-4.417119	5.977373	-1.163099
201	1	0	-1.592937	4.038773	0.886287
202	6	0	-1.437863	2.205555	2.060382
203	8	0	-0.811727	1.133100	2.308786
204	8	0	-2.650792	2.366379	2.700682
205	6	0	-3.604792	3.413361	2.304149
206	1	0	-3.853113	3.325556	1.235613
207	1	0	-4.492771	3.217720	2.907486
208	1	0	-3.211298	4.407215	2.532797
209	6	0	1.045401	5.212796	1.413968
210	6	0	0.293092	4.313677	2.260245
211	1	0	0.555370	6.150916	1.145520
212	1	0	0.872804	3.500679	2.704897
213	6	0	2.412238	5.085835	1.029829
214	6	0	3.035978	6.142538	0.272415
215	6	0	3.254375	3.975567	1.395939
216	6	0	4.373818	6.103548	-0.089905
217	1	0	2.429515	7.000211	-0.014763
218	6	0	4.597641	3.935953	1.047080
219	1	0	2.837597	3.153144	1.971164
220	6	0	5.171025	4.994972	0.297471
221	1	0	4.831936	6.903761	-0.661508
222	1	0	5.232818	3.108107	1.344165
223	7	0	6.555857	4.945862	-0.070993
224	8	0	7.265446	3.918086	0.289620
225	8	0	7.060059	5.922804	-0.753416
226	6	0	-0.584850	4.997052	3.261995
227	6	0	-0.826332	4.553561	4.515790
228	1	0	-1.017069	5.948571	2.939572
229	1	0	-1.444706	5.116994	5.210719
230	1	0	-0.398622	3.623996	4.886781

ET2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.106483	1.212184	-3.370403
2	6	0	-2.493430	1.323246	-2.119837
3	6	0	-1.142990	1.805869	-2.145884
4	6	0	-0.510550	2.105402	-3.371159
5	6	0	-1.162892	1.971376	-4.619657
6	6	0	-2.475991	1.531487	-4.579879
7	1	0	0.511962	2.478582	-3.367567
8	1	0	-0.666507	2.216779	-5.551108
9	6	0	-3.365909	1.118010	-0.907872
10	6	0	-3.345636	0.046104	0.052290
11	6	0	-4.411052	2.036759	-0.752796
12	6	0	-4.337413	-0.016422	1.057396
13	6	0	-5.387310	1.952720	0.249299
14	6	0	-5.381193	0.928814	1.178818
15	1	0	-4.315383	-0.821651	1.788422
16	1	0	-6.132396	0.849962	1.955185
17	8	0	-4.424373	0.763311	-3.625636
18	8	0	-3.357819	1.322053	-5.661202
19	8	0	-6.329661	2.988212	0.113083
20	8	0	-4.683907	3.150550	-1.582457
21	6	0	-4.678429	1.090401	-5.042353
22	6	0	-5.782579	3.885592	-0.919892
23	1	0	-5.374782	4.790316	-0.432181
24	1	0	-6.558537	4.105645	-1.653682
25	1	0	-5.158043	0.239308	-5.527276

Anexo VI: Computational methods

26	1	0	-5.268586	2.013002	-5.098112
27	15	0	-0.183425	1.965701	-0.525078
28	15	0	-1.948698	-1.243205	0.135846
29	29	0	0.148496	-0.277890	0.351154
30	6	0	1.392970	2.816758	-1.049147
31	6	0	2.382431	2.036620	-1.649914
32	6	0	1.618530	4.169647	-0.809242
33	6	0	3.623216	2.586694	-2.008557
34	1	0	2.217068	0.968405	-1.844938
35	6	0	2.847440	4.769723	-1.129682
36	1	0	0.845950	4.796213	-0.348060
37	6	0	3.856446	3.935570	-1.658648
38	6	0	-1.060622	3.334971	0.365091
39	6	0	-1.070541	3.295056	1.753768
40	6	0	-1.668370	4.383213	-0.327915
41	6	0	-1.651283	4.336999	2.499676
42	1	0	-0.624993	2.445853	2.300458
43	6	0	-2.240617	5.459755	0.362183
44	1	0	-1.695653	4.371889	-1.421993
45	6	0	-2.160385	5.437102	1.778199
46	6	0	-2.437407	-2.200496	1.661798
47	6	0	-3.421946	-3.191186	1.600475
48	6	0	-1.822798	-1.898112	2.872975
49	6	0	-3.771387	-3.936355	2.733137
50	1	0	-3.933623	-3.408136	0.655087
51	6	0	-2.139623	-2.608914	4.045516
52	1	0	-1.068202	-1.096209	2.947784
53	6	0	-3.052366	-3.676550	3.925343
54	6	0	-2.296982	-2.538709	-1.152077
55	6	0	-1.749786	-3.805340	-0.907711
56	6	0	-3.049497	-2.307322	-2.294112
57	6	0	-2.033179	-4.889270	-1.744250

Anexo VI: Computational methods

58	1	0	-1.109064	-3.976429	-0.033636
59	6	0	-3.337656	-3.359111	-3.193415
60	1	0	-3.445032	-1.310115	-2.523289
61	6	0	-2.901443	-4.648947	-2.840399
62	7	0	2.108953	-0.564049	0.673367
63	6	0	3.135621	-1.170318	-0.007261
64	6	0	2.638853	-0.094425	1.941412
65	1	0	4.088637	-0.617090	-0.087889
66	6	0	2.916748	-2.086706	-1.149841
67	6	0	4.010756	-2.401378	-1.996255
68	6	0	1.665676	-2.692334	-1.421672
69	6	0	3.856028	-3.280922	-3.081355
70	1	0	4.982324	-1.952169	-1.800316
71	6	0	1.506048	-3.559075	-2.514807
72	1	0	0.822016	-2.478415	-0.769257
73	6	0	2.600549	-3.860383	-3.351205
74	1	0	4.708419	-3.508810	-3.716888
75	1	0	0.527837	-3.998052	-2.717031
76	1	0	2.476107	-4.532868	-4.196901
77	6	0	-1.418373	-6.263609	-1.437579
78	6	0	-2.465602	-7.114973	-0.693852
79	1	0	-3.356828	-7.292497	-1.313041
80	1	0	-2.058811	-8.094776	-0.424661
81	1	0	-2.800105	-6.625007	0.235667
82	6	0	-0.972124	-6.962900	-2.732977
83	1	0	-1.821643	-7.173238	-3.398658
84	1	0	-0.272337	-6.341713	-3.301075
85	1	0	-0.477983	-7.916146	-2.524377
86	6	0	-0.172191	-6.139375	-0.532893
87	1	0	0.613444	-5.535154	-1.002583
88	1	0	-0.403937	-5.690875	0.438848
89	1	0	0.264614	-7.124338	-0.333944

90	6	0	-4.044959	-2.970360	-4.500593
91	6	0	-3.109182	-1.988364	-5.240887
92	1	0	-2.898728	-1.088450	-4.655237
93	1	0	-2.146335	-2.461310	-5.466223
94	1	0	-3.540131	-1.660062	-6.191532
95	6	0	-4.329446	-4.132166	-5.464947
96	1	0	-5.158825	-4.758145	-5.126315
97	1	0	-4.593128	-3.763704	-6.461756
98	1	0	-3.452479	-4.785438	-5.578197
99	6	0	-5.384812	-2.289170	-4.150959
100	1	0	-5.958940	-2.057907	-5.052445
101	1	0	-6.005667	-2.935471	-3.523155
102	1	0	-5.234179	-1.349378	-3.601600
103	6	0	-2.916916	6.589793	-0.427487
104	6	0	-1.678183	4.196082	4.029365
105	6	0	-0.403056	4.852807	4.596327
106	1	0	0.497424	4.351579	4.225370
107	1	0	-0.336069	5.914211	4.317842
108	1	0	-0.383853	4.797047	5.689314
109	6	0	-1.685034	2.706009	4.440155
110	1	0	-2.569091	2.189976	4.051555
111	1	0	-0.799856	2.162894	4.071058
112	1	0	-1.689971	2.598104	5.528979
113	6	0	-2.939317	4.830801	4.638637
114	1	0	-3.844916	4.446704	4.155550
115	1	0	-3.015545	4.619012	5.709144
116	1	0	-2.962531	5.919160	4.517531
117	6	0	-1.983793	7.815405	-0.464228
118	1	0	-2.439260	8.641948	-1.019294
119	1	0	-1.761494	8.187566	0.545978
120	1	0	-1.031156	7.577944	-0.947609
121	6	0	-4.264459	6.956763	0.219962

122	1	0	-4.132085	7.316524	1.252368
123	1	0	-4.779511	7.744991	-0.334647
124	1	0	-4.929456	6.081884	0.275476
125	6	0	-3.200516	6.177621	-1.891032
126	1	0	-2.278817	6.080297	-2.474979
127	1	0	-3.728186	5.218335	-1.956406
128	1	0	-3.815722	6.928679	-2.396583
129	6	0	3.032599	6.272382	-0.876421
130	6	0	3.691387	6.450281	0.506149
131	1	0	3.066806	6.035286	1.302638
132	1	0	4.668185	5.945212	0.549683
133	1	0	3.861504	7.507849	0.730561
134	6	0	1.671122	7.006338	-0.872804
135	1	0	1.159977	6.890799	-1.834839
136	1	0	1.002445	6.635272	-0.087390
137	1	0	1.807953	8.079125	-0.702360
138	6	0	3.887767	6.926117	-1.974595
139	1	0	3.934807	8.012021	-1.856810
140	1	0	4.920755	6.551206	-1.970326
141	1	0	3.486432	6.711690	-2.970797
142	6	0	4.644885	1.698843	-2.734556
143	6	0	3.925692	0.605055	-3.555406
144	1	0	3.300797	-0.047127	-2.932351
145	1	0	3.285543	1.041895	-4.328049
146	1	0	4.648929	-0.044669	-4.060792
147	6	0	5.498262	2.505304	-3.728203
148	1	0	4.870455	3.095670	-4.403823
149	1	0	6.165482	3.215736	-3.224822
150	1	0	6.126246	1.849879	-4.339319
151	6	0	5.538158	1.030618	-1.671887
152	1	0	6.073714	1.778932	-1.069400
153	1	0	4.951127	0.404530	-0.980962

154	1	0	6.294470	0.387668	-2.135286
155	8	0	5.118520	4.492792	-1.910317
156	8	0	-3.274535	-5.741894	-3.635074
157	8	0	-3.325398	-4.471160	5.048052
158	8	0	-2.702857	6.525193	2.478381
159	6	0	-1.729471	7.515332	2.894206
160	1	0	-1.319300	8.019037	2.005870
161	1	0	-2.335262	8.202205	3.495247
162	1	0	-0.934862	7.050221	3.497827
163	6	0	-2.420200	-5.594251	5.201352
164	1	0	-2.758129	-6.041026	6.142581
165	1	0	-2.551503	-6.290370	4.359061
166	1	0	-1.380502	-5.239325	5.277297
167	6	0	-1.467804	-2.191340	5.362526
168	6	0	-1.119751	-0.687031	5.344024
169	1	0	-0.458143	-0.415429	4.507320
170	1	0	-2.020907	-0.071181	5.255767
171	1	0	-0.606304	-0.389098	6.263129
172	6	0	-2.392331	-2.415967	6.571684
173	1	0	-2.572688	-3.479307	6.767976
174	1	0	-1.969347	-1.983740	7.483124
175	1	0	-3.374887	-1.960318	6.408128
176	6	0	-0.167923	-3.005828	5.513120
177	1	0	0.350137	-2.757331	6.444601
178	1	0	-0.370313	-4.087132	5.526548
179	1	0	0.524128	-2.810616	4.687134
180	6	0	-4.890217	-4.982457	2.631023
181	6	0	-5.826428	-4.686333	1.435660
182	1	0	-6.294886	-3.701089	1.531482
183	1	0	-5.297742	-4.717763	0.476941
184	1	0	-6.634009	-5.424099	1.382971
185	6	0	-5.764239	-4.980573	3.896818

186	1	0	-5.195467	-5.286058	4.786982
187	1	0	-6.158212	-3.980996	4.106942
188	1	0	-6.612484	-5.663736	3.801941
189	6	0	-4.246246	-6.364836	2.415598
190	1	0	-5.004480	-7.148859	2.331921
191	1	0	-3.637261	-6.385663	1.496400
192	1	0	-3.586291	-6.635553	3.253018
193	6	0	-4.548645	-6.322914	-3.251082
194	1	0	-4.716048	-7.062151	-4.042409
195	1	0	-4.443195	-6.810204	-2.269024
196	1	0	-5.334838	-5.562735	-3.239505
197	6	0	6.055461	4.329149	-0.815401
198	1	0	6.964234	4.794715	-1.213160
199	1	0	5.687286	4.866176	0.071538
200	1	0	6.214782	3.259202	-0.609859
201	1	0	3.517905	0.566241	1.814644
202	6	0	1.590391	0.614621	2.778606
203	8	0	0.359864	0.483961	2.595909
204	8	0	1.979072	1.410490	3.834690
205	6	0	3.379322	1.795945	4.079582
206	1	0	3.765186	2.396868	3.247615
207	1	0	3.339778	2.400379	4.986907
208	1	0	4.012569	0.918885	4.244142
209	6	0	3.917205	-2.272119	1.675934
210	6	0	3.188631	-1.423113	2.694324
211	1	0	3.444996	-3.211720	1.392109
212	1	0	3.839110	-1.143342	3.533233
213	6	0	5.345213	-2.211633	1.605867
214	6	0	6.181363	-3.088272	0.934955
215	1	0	5.728576	-3.966244	0.473067
216	1	0	2.314721	-1.947019	3.096784
217	1	0	5.801988	-1.337266	2.080106

218	6	0	7.616748	-2.955575	0.787906
219	6	0	8.341390	-3.951079	0.059132
220	6	0	8.375335	-1.867897	1.331195
221	6	0	9.720557	-3.873803	-0.125826
222	1	0	7.792436	-4.790551	-0.362270
223	6	0	9.753115	-1.777799	1.154934
224	1	0	7.872261	-1.089286	1.896662
225	6	0	10.429016	-2.780926	0.422092
226	1	0	10.264149	-4.630832	-0.680485
227	1	0	10.325423	-0.953452	1.566297
228	7	0	11.862585	-2.683673	0.231639
229	8	0	12.485568	-1.672704	0.737056
230	8	0	12.462182	-3.609012	-0.436930
