

Apéndice de Estudio computacional de los procesos de absorción, fluorescencia, fosforescencia y entrecruzamiento de sistemas del trimetil éster de clorina e6 y sus derivados con zinc y piridina.

Marlon D. Suárez Ruiz,^{*a} Martha C. Daza,^a y Markus Doerr^a

22 de mayo de 2025

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A. Geometrías optimizadas

En esta sección se muestran las geometrías optimizadas de los estados basal y excitados para el trimetil éster de clorina e6 (TMEe6) y sus derivados con zinc (ZnTMEe6) y con piridina (PyrTMEe6). Calculados con TD-DFT CAM-B3LYP(CPCM)/def2-SVP. Los estados tripletes fueron optimizados usando la aproximación de Tamm-Dancoff (TDA).

S1. Trimetil éster de clorina e6 (TMEe6):

S1.1) Estado basal optimizado, S₀

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Coordinates from ORCA-job opt		
C	-5.05715986860763	0.93639262679593
C	-4.40056425967159	2.10789469444938
N	-2.82466453062635	0.51924968459622
C	1.49602569952630	3.20588585181840
H	-0.82091258071643	5.46005532103585
C	-2.97441060805000	1.83487521725581
H	-4.32997175477249	3.99234763595533
H	-5.12169378268758	4.06441118290524
C	-4.04766737511535	-0.08956270927356
C	1.32962457797726	3.56966116349732
H	0.80510289857914	3.71738077257023
C	-1.25593604280525	-3.32547794170118
H	-1.43438688301568	-0.23624522866625
C	-4.22912913925529	-1.41625980673435
C	6.35953746172677	-0.61265985516565
C	4.57352352275562	1.96492597546208
C	-3.19851253300534	-2.38037985511850
O	0.65064977817226	0.95539908132844
H	-2.94730111296384	0.04070443706176
N	-1.88494121713057	-2.11519704042209
C	-2.22608321053342	-4.40105121843796
H	-5.38712320747966	-3.96464051311629
C	-3.45421096022617	-3.80117269715749
H	-4.73274790217948	-5.49986314148885
H	3.64898245126824	2.12851229527382
C	-4.80683050747627	-4.42357727229518
H	-5.39813409195780	-4.30115842469705
H	0.44759203353801	-4.55938542801501
C	-1.90599491926631	-5.85952881885410
H	-2.59162278471581	-6.46621918812624
H	-1.45998522407022	-7.61408031216150
H	-0.85963574843269	-6.08321271092490
O	5.74374949546305	2.23417820595151
C	-1.69148112370156	-6.54623357602128
H	-2.72333497954610	-6.36383155979352
H	-1.00769200615519	-5.99306585764488
C	-6.49142510954874	0.66847207178479
H	-6.79210495997079	-0.36366748317468
H	-5.25601804133910	-1.76725409835646
C	-7.44352633400184	1.55023657245800
C	3.73989051328679	1.34407732828208
H	-0.86794713940938	3.59582472691703
C	-4.98148937967699	3.43805396115013
H	-5.96497257919685	3.32268653628035
H	-0.02366662247639	3.70095931731837
C	-1.96008672906128	2.76614015344778
H	0.70638043800579	5.86276790215243
H	-8.49198242295828	1.24505412581836
C	-0.59049569088389	2.58249663857580
C	-0.21358973316215	1.74834025358174
H	-7.21931106654390	2.58633705447285
C	0.11272249288664	-3.52564369184567
C	2.37236013268866	0.81158935003504
C	4.58576797962432	2.88100567718197
C	3.18940896527797	-1.64546771150976
O	3.88113612212125	2.24556400597006
C	1.14095659076867	-2.58941404957817
		0.49790246490037
		0.79532469617562
		0.43992889721721
		-0.17021665498904
		1.29231082292723
		0.73371687146302
		1.82837284048100
		0.24334109543759
		0.28778282599028
		-1.65985225845567
		1.77344951377572
		-0.17012941688541
		-3.80647969266040
		0.00207803375814
		1.70738527499351
		0.71572002836776
		-0.13198218998506
		-2.89223255496360
		-2.86762117781670
		-0.04507811654115
		-0.35548309740192
		-1.28193623402277
		-0.33541151607472
		-0.67142569247923
		-1.14769097840031
		-0.46599362010704
		0.45553856767334
		-0.20717579087571
		-0.47949665767929
		1.49989749669926
		0.74133583084062
		1.42385101369742
		0.58889312132035
		0.87209101417093
		-1.01694007159370
		-1.10256614513229
		0.41015290771016
		0.61640534209192
		-0.09732131816769
		0.08754777578609
		-0.38253833947802
		-1.78586360547175
		1.13935311689355
		1.61477428083447
		-3.32100001313978
		0.89611768889629
		0.49140097398400
		0.05317539836597
		0.68671436165807
		-2.60510466932133
		-0.17269696910479
		-0.12200394333648
		-0.02520864236051
		2.87713452819329
		0.17863066711794
		1.81629936150548
		0.01140499111915

H	5.37211153974257	2.22088057095856	3.26853207110702
H	5.04577286568917	3.81697835753995	2.53177774183140
N	0.03058492368771	1.43567041355214	0.39468208476183
C	1.33424378848043	1.71399093636571	0.07597363505343
C	-1.85261401998448	0.07687641886743	-2.84017390315677
C	0.38922536225551	3.74240271081484	0.74928560340674
H	4.36846743511318	0.58214453790990	-0.85658397581317
H	-2.28283691037003	3.77834120653529	1.13230050261979
H	1.48035303200064	4.65456233673043	-1.75929130197748
H	-0.65987416113959	5.24019844859400	-0.46110325092511
N	1.00344472051227	-1.21887077975414	0.05314168533905
C	-0.12970617596517	5.14793579311328	0.49633940251626
C	2.52855274634809	-2.87275976211377	0.08553483427180
H	2.40226651158894	-5.01911392708017	0.25053366751242
H	3.66370114850302	-4.42546308810023	-0.85863317667979
H	2.47316713499676	3.57607497611730	0.15565313233298
C	2.21008240182942	-0.60184823353100	0.11466905604840
C	0.00313831703419	3.21489837774976	-2.33092147830168
H	-1.48507612139179	-0.58869494056914	-2.04741080335734
C	4.63806967261152	-1.58935715231162	0.44628850296131
H	6.44400896570129	0.14662587891935	2.49074769070853
C	3.14814624867390	-4.23067505566064	0.09333090505108
H	3.90979215473087	-4.31234658336405	0.88120085217978
H	3.84500942163979	3.08552343536388	3.65763642409201
H	6.69007216896198	-1.59041174433669	2.08198214230356
H	6.97289071777812	-0.32688065090950	0.84293581615514
O	-1.50689597195870	1.42930719928115	-2.55531046277586
O	4.97999237531018	-0.66178565138355	1.34765764953574
H	2.13951619115599	3.09459395367847	-2.23303575538814
O	5.44390695191708	-2.36082394560238	-0.02227439146342
H	-1.94562070147669	0.01345142044792	0.34703830485835
H	0.12315827475076	-0.71248308892600	-0.01427564240921

S1.2) Primer estado single optimizado, S₁

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Coordinates from ORCA-job opt

C	-5.08488399462605	0.94950962600534	0.35751461482436
C	-4.41970867266576	2.14462485673058	0.64103108230817
N	-2.86279130422016	0.52986451985498	0.37075400158820
C	1.49488961284484	3.20603594859222	-0.13010336918417
H	-0.82334688575675	5.45096352808530	1.34682305296839
C	-3.01600819168322	1.86282801414634	0.63976636431798
H	-4.26373915638186	4.28517744661152	0.83528395308543
H	-5.77532770180702	3.71859964309667	0.09515197929019
C	-4.07639636500305	-0.06697440203331	0.19263103626399
C	1.34753582613846	3.60378396631173	-1.61500892945469
H	0.78570757575324	3.68385568171621	1.81230242509466
C	-1.26701899266288	-3.30443289017901	-0.13103976762484
H	-1.26624860815074	-0.25458543267997	-3.83817361194122
C	-4.24611119638273	-1.43295693862553	-0.06691446306153
C	6.38232732602851	-0.64420364764533	1.65799337282497
C	4.57251799466191	1.95074563333712	0.76310624966178
C	-3.21998418473263	-2.36785283616547	-0.15005025984156
O	0.76248363106855	1.00241186335243	-2.87642715616949
H	-2.80891972597668	-0.01870879102909	-2.93736728173998
N	-1.88878912194407	-2.10246177812654	-0.03626670435531
C	-2.24240150114519	-4.40067327665397	-0.32023341276939
H	-5.36251029109324	-3.98110568989856	-1.33535968551346
C	-3.46238805878101	-3.81136642507775	-0.34000421021447
H	-4.74003685515446	-5.51011373524849	-0.66977489426975
H	3.66005537615804	2.15947105851463	-1.10239689345557
C	-4.81110482879999	-4.42880377155311	-0.49365849743101
H	-5.42475907130556	-4.27390894308275	0.40808058249602
H	0.44663320921060	-4.55090407918093	-0.15544680336007
C	-1.90142505155333	-5.85462308776651	-0.41315410252183
H	-2.53566126554318	-6.42779870663971	1.59201349876434
H	-1.38591858466514	-7.56348653078002	0.84178994000779
H	-0.81528647856993	-6.00197776514180	1.47771654833467
O	5.74209487299803	2.22932943067201	0.65502114071407

C	-1.64378595817295	-6.49957653984187	0.95173160048271
H	-2.72278255706312	-6.38567720057102	-0.91696173497891
H	-1.01477954767875	-5.98617097191393	-1.05352952165171
C	-6.50707294594276	0.67774163697656	0.22002183426983
H	-6.75095840575122	-0.29845345337459	-0.21036392181958
H	-5.26635275950811	-1.79645193660416	-0.17578035063672
C	-7.53608158951639	1.47001536254876	0.55599115706971
C	3.74907289274580	1.35549701259899	-0.35727977075607
H	-0.84672783093652	3.58391893584651	-1.76370996481579
C	-5.02091915624864	3.49168579607041	0.86401048589992
H	-5.53048061894798	3.55498804372335	1.83968004392609
H	0.00877370889575	3.73916730587185	-3.28905585640269
C	-1.97281340451129	2.78328429563602	0.83095545232335
H	0.71615499470387	5.85425875163582	0.57036980334477
H	-8.56194610645330	1.13410591702199	0.38830928761826
C	-0.61114296748423	2.58976378767205	0.67926522156353
C	-0.13303895673217	1.76682382280582	-2.60668358795577
H	-7.40701182749177	2.45142161432942	1.01233274690235
C	0.10705301299646	-3.51890217968567	-0.08062340087391
C	2.38517400827815	0.80878727084698	-0.02091116653839
C	4.55587220044869	2.81007602158411	2.94816869117437
C	3.19705263419275	-1.64796187456804	0.14558971136657
O	3.86650344323512	2.19856278378103	1.86325125558343
C	1.12561859900520	-2.56698560513551	0.02887693415568
H	5.34761908502821	2.14764995687285	3.32461070680193
H	5.00576683078474	3.76170672636669	2.63372827923937
N	0.03353515985949	1.42384856742086	0.39099982135634
C	1.32076345740805	1.71553449552699	0.08656809493852
C	-1.71673012693275	0.04857267504824	-2.88331381674156
C	0.37658993300070	3.73313708627559	0.78629031637878
H	4.38234224724505	0.60901216555866	-0.85034621338141
H	-2.28733837458997	3.79813787293554	1.06564549236505
H	1.47874700632868	4.69317597743030	-1.68314378305072
H	-0.64479493793909	5.25885932146862	-0.40857273418534
N	0.99492135999132	-1.20437684738684	0.08216548786519
C	-0.12607996416971	5.14699349435003	0.55320560324500
C	2.52589736034584	-2.86224337483567	0.06768348234522
H	2.66938632364787	-4.83300910471075	0.90918110419051
H	2.81927745573818	-4.77540211790340	-0.85259743352185
H	2.47223415824672	3.56050742784967	0.21273459645070
C	2.21713638909188	-0.58693256248447	0.11169145656351
C	0.03822427180987	3.23480875844432	-2.30837573893097
H	-1.34997688768998	-0.60368323977225	-2.07914336226696
C	4.65441314232324	-1.57558612356547	0.37028282239567
H	6.46765521957133	0.07431989197713	2.47880637495772
C	3.08414524266775	-4.24479938471202	0.07599035965599
H	4.17593486564671	-4.23258271155411	0.15450146525183
H	3.80733647837478	2.98239983709766	3.72903206238797
H	6.73928835350260	-1.63375456249482	1.97286364154820
H	6.97036143337665	-0.30005680742079	0.79749340079491
O	-1.41656294166192	1.41121034444625	-2.59393688151452
O	4.99568692166583	-0.70376652959473	1.32528037066837
H	2.17581605749095	3.15803211741082	-2.18492170526408
O	5.46811981698879	-2.28335575993935	-0.17879934868100
H	-1.98566871499533	0.01345590159760	0.32420710699793
H	0.11881117952345	-0.68582257847725	0.04774422225206

S1.3) Segundo estado single optimizado, S₂

89			
Coordinates from ORCA-job opt			
C	-5.07022260253030	0.94133166851166	0.45879281275563
C	-4.38982689056111	2.14190125318011	0.74378177910815
N	-2.85088269377190	0.53148718178499	0.40398448055821
C	1.50805486089613	3.20967499480692	-0.17364262565275
H	-0.80359861051041	5.48372247334391	1.26540822159131
C	-3.00136536837497	1.85711486085297	0.69641559758366
H	-4.22607208358801	4.25638507235835	1.13771880845398
H	-5.66418075582991	3.78977107205757	0.20893146160245
C	-4.07026294399898	-0.06158720723810	0.24950131410968

C	1.34827042339712	3.56302763083687	-1.66613534418002
H	0.83086127248524	3.74460217005856	1.76726003378177
C	-1.26269679945534	-3.31612375566276	-0.19750991619965
H	-1.32102825903065	-0.29032851880582	-3.84267547693137
C	-4.23474342589772	-1.42284770591302	-0.04468458659304
C	6.35401946609016	-0.56969045174074	1.75270438010936
C	4.56654342751072	1.96846577949750	0.70337396841616
C	-3.21139793110750	-2.36365860800227	-0.17335805355068
O	0.72927913754994	0.92715907363544	-2.86455031196328
H	-2.86102347089863	-0.02954325513376	-2.94432638001857
N	-1.88449780427153	-2.10410725540873	-0.06862184023025
C	-2.24240001304047	-4.39159948542413	-0.40555186262604
H	-5.38456990976987	-3.92875981245556	-1.36207494517815
C	-3.46330062310800	-3.79160891519715	-0.39613706139989
H	-4.74709360696026	-5.47887814316552	-0.76691095457125
H	3.64270057993122	2.09764504214293	-1.16534213217341
C	-4.81594220361955	-4.40508178162942	-0.54799749187694
H	-5.41390406046725	-4.28864958372114	0.37000245378168
H	0.42387241695428	-4.57288414005514	-0.22892781232090
C	-1.92194532872667	-5.84877975907259	-0.53413226715405
H	-2.60656514158947	-6.46337611631447	1.44192509163037
H	-1.46479598769159	-7.60191640094801	0.68392748326429
H	-0.87679495228748	-6.06819991588690	1.37104905472465
O	5.73090538759555	2.25278461174628	0.57096187976541
C	-1.70410065181875	-6.53613278878656	0.81660819576688
H	-2.74073497040935	-6.35243736394284	-1.06965414475432
H	-1.02516564891959	-5.97942564870947	-1.16020604907070
C	-6.49612851529450	0.67195387855837	0.37082807908700
H	-6.75166035369615	-0.34667944775337	0.06388837533219
H	-5.25707366035452	-1.78413189848611	-0.15089950643654
C	-7.51956225794948	1.50332224634873	0.61856072230461
C	3.73860245263786	1.32366370808743	-0.38995511491123
H	-0.84712212967070	3.55265689023282	-1.80722687659121
C	-4.99111010158239	3.47885663372668	1.02299844535413
H	-5.59093790028313	3.46426552704033	1.94682005642208
H	0.00448899753279	3.66024087340835	-3.33846097576417
C	-1.94086448173794	2.78264256266485	0.86130814714933
H	0.72689062076969	5.87762420235297	0.46723839205706
H	-8.54712887195399	1.15031617702401	0.50632945782894
C	-0.58483341117384	2.60867735757998	0.68958223631212
C	-0.15442828724431	1.71037403304293	-2.61046649279497
H	-7.38662819780141	2.53621492508095	0.93848386174330
C	0.09941769051826	-3.53635144264149	-0.14159460694882
C	2.37886221943909	0.79875511135297	-0.02103347875481
C	4.55286800126313	2.91525547818592	2.85326673286617
C	3.19379923673433	-1.65599452441465	0.24032866582167
O	3.86681907367533	2.24853986980659	1.79830700884271
C	1.15103445881945	-2.60195569706173	0.01128379043898
H	5.34095791156232	2.27221962509597	3.26864234187337
H	5.00535152437139	3.84814878810508	2.49071020237112
N	0.05837218720987	1.43919585125105	0.42346618295106
C	1.33623323231721	1.71908196859327	0.08723620976425
C	-1.76788068921151	0.01741390432948	-2.88752784616071
C	0.40562307320859	3.75894914434538	0.74670163336445
H	4.36745057791641	0.55014083176617	-0.84405467745351
H	-2.26030280660375	3.79860972885651	1.09002650293735
H	1.48308976561077	4.64956681815990	-1.76927332399806
H	-0.63483582056432	5.24175670780821	-0.48471613257472
N	1.01082593995325	-1.23580925188736	0.04062325031689
C	-0.10854693170631	5.16216196188409	0.47636022297392
C	2.52470781971432	-2.89235290042364	0.12962168707708
H	2.37608407899860	-5.03691375034759	0.27272782377289
H	3.71285772163881	-4.45132819203945	-0.74876903561968
H	2.48637437147329	3.57808369364100	0.15087388520895
C	2.22110580003007	-0.61870443721362	0.14167837294001
C	0.03346445180365	3.18259634617088	-2.34427332090025
H	-1.41594040001523	-0.64525577700280	-2.08529110179736
C	4.63210761338701	-1.60303899153404	0.54019378772444
H	6.44795475957845	0.24881249449173	2.47247185227981

C	3.13649426293025	-4.25335574066424	0.16729189962403
H	3.84437533261941	-4.34640518909106	1.00304136437329
H	3.80054735569363	3.12883724606416	3.62007089331232
H	6.65964263746157	-1.52069896995905	2.20859664956698
H	6.98340679214235	-0.36896274154815	0.87559516698026
O	-1.44378801627336	1.37417865418552	-2.59412906388635
O	4.97781801590356	-0.61945723221120	1.38153877341270
H	2.16980343709069	3.09956093148712	-2.23229938960197
O	5.43580601797947	-2.41735939888601	0.14291130937318
H	-1.97612547181646	0.01455515230843	0.32134537109953
H	0.12798463877339	-0.73575801147219	-0.04407617122211

S1.4) Tercer estado single optimizado, S₃

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Coordinates from ORCA-job opt

C	-5.08836597850229	0.94915121060372	0.43802227242264
C	-4.42252712793748	2.13363947957990	0.72185298219498
N	-2.85428592020009	0.52658534320948	0.42302706776540
C	1.48581106427037	3.22473920007296	-0.13455730992839
H	-0.84888852856987	5.47207859590766	1.31244897996838
C	-3.01039900909119	1.85283237294506	0.69398431442822
H	-4.31608377727307	4.10817462411225	1.57582513147104
H	-5.29499229750923	4.00765425954613	0.09972175042914
C	-4.07819562843313	-0.07832997864529	0.26244633361435
C	1.33763150345001	3.60606332579470	-1.62426210296872
H	0.77766501226217	3.72769543311163	1.80269637942869
C	-1.27037532033565	-3.32113523284739	-0.12490522919346
H	-1.25543340578613	-0.28362612758135	-3.81502217784456
C	-4.25147117645550	-1.42133120563343	-0.00663491192757
C	6.40172179192114	-0.65134111992757	1.61335559169458
C	4.55849037307132	1.94638479641153	0.76883928885071
C	-3.2240126906529	-2.38911808367688	-0.11129433784407
O	0.76383927133416	0.98926749014705	-2.86929369840341
H	-2.80558594374617	-0.04178022976287	-2.92828058573292
N	-1.89263955909404	-2.11828732096631	-0.01466956209428
C	-2.22554364257407	-4.40048177425454	-0.30375553664050
H	-5.40010065689917	-3.98622436162964	-1.24699620797626
C	-3.46733769966567	-3.80424864795920	-0.29822394589962
H	-4.72893757081265	-5.51437855771372	-0.63857526300835
H	3.64612410758504	2.18296704372977	-1.09533242408737
C	-4.81328679726729	-4.43881965048470	-0.43111376439054
H	-5.41103003982588	-4.32612012701179	0.48887120137328
H	0.47628975362158	-4.54402507947427	-0.15623714827991
C	-1.89372118307086	-5.85686414673170	-0.41092640924772
H	-2.55557247415133	-6.45183698212193	1.57947148267747
H	-1.41444746459231	-7.59482406413661	0.82585547107094
H	-0.82893010988633	-6.04827433484548	1.48657010190993
O	5.72729183813332	2.22781110858709	0.66613649761329
C	-1.65897915087356	-6.52814955384287	0.94593824848469
H	-2.71131932291388	-6.37717048125592	-0.93366047624967
H	-0.99947330954008	-5.99258742645307	-1.04113568478330
C	-6.51511903765719	0.68028000081654	0.34038169595280
H	-6.79815479155359	-0.37235309128168	0.44263853873608
H	-5.27666578631122	-1.77465638677517	-0.11781544484577
C	-7.49717990504354	1.56793822336820	0.12871339895107
C	3.73695898238382	1.36783748981334	-0.36326203902909
H	-0.85687965469045	3.57369782484786	-1.77636730271200
C	-5.01512563626427	3.46951911970777	1.02055143262650
H	-5.92953689916155	3.36345439666944	1.62187883780300
H	0.00119975095930	3.71701631667943	-3.30124425950733
C	-1.97861468100514	2.78363805236670	0.86648247641961
H	0.68774369415756	5.87914603472097	0.53245221925988
H	-8.53702306901581	1.23649851542968	0.08248017685954
C	-0.61298040639359	2.60431668530411	0.69518764113455
C	-0.13409106506588	1.75164860498921	-2.60193548580510
H	-7.31004007859493	2.63155537625817	-0.02392868375017
C	0.12809635111772	-3.51355248516760	-0.08284000119108
C	2.37456930532270	0.81847002506991	-0.03002245072269
C	4.53759204748991	2.75418085861390	2.97302810764953

C	3.20170107572063	-1.63141188766824	0.11376228590429
O	3.84996345415790	2.17007255993576	1.87141121672049
C	1.13197908194385	-2.56447185760000	0.01920734873482
H	5.34062982949857	2.09016956321252	3.32143723812662
H	4.97177744038667	3.72231404352978	2.68819321830803
N	0.03454328573779	1.44539745230018	0.41540911023621
C	1.31451418055885	1.73414368383380	0.09334041045816
C	-1.71380760751906	0.02605310255640	-2.86611833196776
C	0.36654937679214	3.75759549120887	0.77559653094722
H	4.36941278053063	0.62813146098026	-0.86747828762377
H	-2.30263007828223	3.79856028082407	1.08987652418203
H	1.46308980498944	4.69553920298767	-1.70423266237760
H	-0.66673882597231	5.25900182235915	-0.44025499565450
N	0.99351442846827	-1.19870035005799	0.08254449407880
C	-0.14804563810930	5.16409900132522	0.52341275889739
C	2.54507012476856	-2.84727582099449	0.04218668850461
H	2.70691880926580	-4.81828916750165	0.87314233518385
H	2.84197764985858	-4.75157568620568	-0.88904836024196
H	2.46149072596100	3.58792433265363	0.20537820565265
C	2.21475007743421	-0.57633403198493	0.09783229368465
C	0.03087279328403	3.22287213686594	-2.31521815341762
H	-1.35432774259150	-0.62114107244392	-2.05426495242108
C	4.66494234995013	-1.54710655889414	0.31101271729164
H	6.48422757713961	-0.00749803126619	2.49451791640479
C	3.11306261250110	-4.22409020867621	0.03972933856365
H	4.20555254828991	-4.20701114587915	0.10956469821835
H	3.79097138656740	2.88968684194945	3.76284350579028
H	6.79102401686780	-1.65465123530462	1.83017199699310
H	6.95993965171661	-0.21230066844467	0.77656450872022
O	-1.41628202125061	1.39103170958360	-2.58368120121813
O	5.00967447319391	-0.71948870025888	1.30191459016642
H	2.16825860684927	3.15888916526106	-2.18978921697163
O	5.47502098283917	-2.21115502091995	-0.29275740422199
H	-1.97762787358777	0.01230375120750	0.35342165868428
H	0.11207061679023	-0.68983751670730	0.06061679893712

S1.5) Primer estado triplete optimizado, T₁

89

Coordinates from ORCA-job opt

C	-5.02869512430476	0.93213332347130	0.51448546163752
C	-4.35926854815124	2.11825967098692	0.85969991622006
N	-2.81406748165525	0.52610600887782	0.44402029484133
C	1.50924329191375	3.16532077596404	-0.20475352452244
H	-0.73776564146010	5.43586224516583	1.34392330610608
C	-2.95764576455019	1.84548306466642	0.79802073415284
H	-4.21917226228513	4.11803196664818	1.64950134251204
H	-5.40741448519886	3.92884169710805	0.34500791338064
C	-4.02817235317587	-0.05026945120318	0.26984541537061
C	1.27748969619315	3.52502311259732	-1.68613829064943
H	0.90239112252034	3.68917005024519	1.76769697550765
C	-1.27025343138464	-3.31061749337987	-0.21951932643376
H	-1.49899223278387	-0.25893321435199	-3.86068295731900
C	-4.20920951373286	-1.42428677510505	-0.08503617614830
C	6.25012571101294	-0.50917903526646	1.96446035300825
C	4.64413481314744	1.95732810382295	0.55695757623473
C	-3.219751138358848	-2.35597739180681	-0.22917847659899
O	0.59396744591166	0.90630733329527	-2.87082041934657
H	-3.00030557180545	-0.02302690504299	-2.89328423277975
N	-1.86240400713411	-2.11677912425803	-0.08795977152428
C	-2.25658956852642	-4.38530933797043	-0.47931024387896
H	-5.35834329137010	-3.87979912834408	-1.52409792621988
C	-3.46953183602364	-3.78243229187637	-0.49670716659703
H	-4.75207064998192	-5.44997685359234	-0.94604623925390
H	3.63649149547593	2.00600616175910	-1.26500647719710
C	-4.82029360366333	-4.38111081255851	-0.70448995175014
H	-5.44419672325984	-4.27973957284390	0.19767424784220
H	0.41989785544578	-4.59759690030892	-0.18281982955135
C	-1.92831101547320	-5.83763397872026	-0.63038579439980
H	-2.61000576519844	-6.49352640535351	1.33306788956372

H	-1.45109493850096	-7.60386082935123	0.55926525939898
H	-0.88508761065380	-6.07650119077543	1.27614539053383
O	5.82113017985826	2.15234824627931	0.37068264938001
C	-1.70465046327924	-6.54386378132575	0.70986742303102
H	-2.74409362801055	-6.33807349636783	-1.17313388274687
H	-1.03010268891278	-5.95027154336954	-1.25844646070806
C	-6.45927136114561	0.66104195560522	0.41841598520731
H	-6.72324236514378	-0.39800411961741	0.34110734195981
H	-5.23749228506199	-1.75859230919395	-0.21551514174186
C	-7.46737179093575	1.54229289501012	0.40819099169286
C	3.74934980561333	1.27326526206783	-0.45176412989345
H	-0.92397520459914	3.51786526881587	-1.71362522411732
C	-4.96194293164518	3.43250966208492	1.22270147389793
H	-5.76811833643914	3.30424003409684	1.96048392527881
H	-0.15385349670553	3.66131390395175	-3.28206817658947
C	-1.91464456295924	2.75072032390437	0.98719615898543
H	0.74892248188128	5.82400003729745	0.46446432759217
H	-8.49906809846262	1.19167807623137	0.33393048601818
C	-0.54125968446413	2.54887068739062	0.73899492947405
C	-0.27660083210408	1.69492708464982	-2.59093027311828
H	-7.31600413525750	2.62037406026913	0.45846245469832
C	0.10695806620088	-3.55674439301110	-0.12141495658896
C	2.38882880149920	0.78692136951095	-0.01144421217698
C	4.76813700603855	3.13177325872419	2.58511068342184
C	3.17628712196728	-1.67691876522498	0.34546468805027
O	4.00241610349777	2.39614673787650	1.63712248858198
C	1.14177740169915	-2.63107076940853	0.04739225293804
H	5.57297078122108	2.51057870181964	3.00091901051074
H	5.21188342618034	4.02098343183128	2.11649518851725
N	0.04172215364196	1.40431665610502	0.41800414371203
C	1.36803269953464	1.68038328833007	0.06914227632873
C	-1.90584061939054	0.02372237220043	-2.88002469192793
C	0.44252446283572	3.70788137350199	0.76282959112643
H	4.34484395423256	0.46660581143333	-0.89508975860020
H	-2.21013048749321	3.75978665817896	1.26795789237833
H	1.41752312502176	4.61049474208192	-1.79250943277865
H	-0.66249510695902	5.19273225455303	-0.41275855597741
N	1.01227486299400	-1.25607015680911	0.03520185338984
C	-0.08713294833469	5.11134193626589	0.51936251274727
C	2.51549846793184	-2.91633497226937	0.23152249292423
H	2.36157559009330	-5.05697025967439	0.40805389029376
H	3.74236575344973	-4.48574773780677	-0.56271884357543
H	2.49947957692084	3.53701486039101	0.07513133159398
C	2.21225964624750	-0.64733230802777	0.18051584400419
C	-0.07103063364201	3.16010670914609	-2.30254930055443
H	-1.51848619379425	-0.65837248466888	-2.11121687541364
C	4.60028507821315	-1.60145909471200	0.70104650125604
H	6.27914849139714	0.28447261200474	2.71770194664270
C	3.12506656988453	-4.27404634301303	0.32314848612524
H	3.79623735469630	-4.34823030041190	1.19040686658594
H	4.07256893539259	3.42706223338503	3.37806045502723
H	6.55532055718648	-1.46681580480909	2.405574440452899
H	6.92046223956846	-0.25810081789205	1.13208623252323
O	-1.56950305942585	1.37226819165141	-2.56559492380575
O	4.89866965044052	-0.57994414287918	1.51431172298002
H	2.06798176871029	3.05401282999609	-2.28895308157044
O	5.42663440654198	-2.42308550564944	0.37159330733120
H	-1.93408495875511	0.02284450716509	0.33953686426705
H	0.13787872457009	-0.75199375016432	-0.09515842525707

S1.6) Segundo estado triplete optimizado, T₂

89

Coordinates from ORCA-job opt

C	-5.07686705618666	0.94752428310401	0.38504511455589
C	-4.41227948636772	2.12828839007066	0.70024527291522
N	-2.85949356088147	0.50718858796942	0.40739945897824
C	1.47869636822130	3.18594084297527	-0.11024806546159
H	-0.80189749901760	5.40838796626867	1.45728081698342
C	-3.00432894718618	1.84056268516089	0.69852377519345

H	-4.31526658705028	4.09366414570499	1.57544677399535
H	-5.26147826105683	4.00876659710019	0.07703298097188
C	-4.07060817491755	-0.07023730629865	0.21965978608438
C	1.29118220436267	3.59951468510103	-1.58565873839697
H	0.81132123665342	3.62884323318328	1.85633709385319
C	-1.25134213353085	-3.29458610258374	-0.09406814273209
H	-1.35495090536032	-0.22607433948715	-3.80935771221744
C	-4.24455349345872	-1.44696310853613	-0.07008750848503
C	6.41897040824700	-0.62771368388466	1.58706676428811
C	4.58527511404861	1.95556267516863	0.69948456085860
C	-3.21275340259340	-2.35797539324376	-0.13834759639301
O	0.67441615866352	1.01186895350278	-2.84942255977865
H	-2.90177718082170	0.01008511480421	-2.91659127331987
N	-1.87876973448893	-2.09139756167449	-0.00780500854173
C	-2.23601475405139	-4.40001384294257	-0.29388148718317
H	-5.32690426696967	-3.98368605176430	-1.36927472986075
C	-3.44935964216862	-3.81434339483619	-0.33625618605080
H	-4.72634052076615	-5.51132907896730	-0.67840282701426
H	3.63726434095252	2.15903162980419	-1.14880471587473
C	-4.79593622791821	-4.42819418586553	-0.51283001818496
H	-5.42701992406804	-4.26105996606937	0.37447445260160
H	0.44180045055899	-4.56217552549307	-0.10835873129257
C	-1.89160255856732	-5.85308884851760	-0.37840803561037
H	-2.54088823243703	-6.42257434056109	1.62300190506626
H	-1.37811021627660	-7.55402362406820	0.88739748428563
H	-0.82177757100214	-5.98750735323198	1.52317084828321
O	5.75376836200177	2.23128274563422	0.57087691801618
C	-1.64257634370616	-6.49111377139807	0.99137204072684
H	-2.70840343971508	-6.38828518935274	-0.88532414122427
H	-0.99978193868325	-5.98443262835192	-1.01142894287496
C	-6.50333214801619	0.68015508474486	0.24912713499129
H	-6.78807977997893	-0.37348243339147	0.33280435411231
H	-5.26253249984199	-1.80521209737178	-0.20272559917927
C	-7.47897435377761	1.57049625059599	0.02670605363879
C	3.74096987419383	1.35710806870284	-0.40326942084037
H	-0.90716676669805	3.57991515355256	-1.67340012235870
C	-5.00518994452224	3.46298554017911	1.00009699527644
H	-5.93373283873177	3.35462064048080	1.57878222809756
H	-0.09503854221854	3.75800737453205	-3.21851545729076
C	-1.96196932108431	2.75741234091329	0.90525395419947
H	0.72033533487487	5.82183141001018	0.65201694331166
H	-8.51774056644389	1.24097351438953	-0.04833743528216
C	-0.60626457584754	2.55750271005260	0.73470708376626
C	-0.21617148358943	1.77541665325938	-2.56164066398679
H	-7.28753994396557	2.63601096581116	-0.10706710499761
C	0.10761299729823	-3.52945039746851	-0.03834472084219
C	2.38618439803280	0.80411192772272	-0.04016145825354
C	4.60911230283999	2.82810831549612	2.87901788179219
C	3.21075463986339	-1.64758824937925	0.13547860636438
O	3.89894389180093	2.21210863788047	1.81042435773022
C	1.13970880418865	-2.57019358737180	0.05578995586373
H	5.41388481711492	2.17143761960507	3.23723541050413
H	5.04569459771361	3.78243521419187	2.55387629067203
N	0.03376169290555	1.39091758728918	0.41741195141030
C	1.31388431413382	1.69363196014045	0.09206941521549
C	-1.80949406469233	0.06819873858588	-2.85370334953948
C	0.38248513416036	3.69883008100002	0.84033333157470
H	4.36717785006268	0.61163107691483	-0.90727323893871
H	-2.27555844101374	3.76936463643620	1.15169384431843
H	1.42160427410841	4.68946773190950	-1.64514363238037
H	-0.66382089509893	5.24576160846250	-0.30504815000348
N	1.00516007134958	-1.21567248637076	0.09351633603899
C	-0.12380016724174	5.11673474441176	0.64279262072566
C	2.54186616406890	-2.86386248870306	0.08374193433396
H	2.66108562900342	-4.83504509626488	0.92276676793551
H	2.85538605048775	-4.77288158527339	-0.83461479755673
H	2.46432615397248	3.53690828218736	0.21106415622935
C	2.22951143242959	-0.59196577064616	0.10251017779891
C	-0.03708278810820	3.23913504230244	-2.24669338232335

H	-1.45344069457616	-0.59661930631961	-2.05459582305884
C	4.67213207603886	-1.56978163086566	0.33331740978385
H	6.51256431885233	0.07542432115741	2.42026797460223
C	3.09843012305098	-4.24646950773675	0.10206052976799
H	4.18806289660255	-4.23693534499221	0.20781852681771
H	3.87751947286629	2.99641816696499	3.67664869645502
H	6.79109806920794	-1.61945644773622	1.87596386816915
H	6.98648066097886	-0.26046387751886	0.72244476527965
O	-1.50116689303142	1.42541200440645	-2.54534592906480
O	5.02693028568161	-0.69433774387114	1.27906918487749
H	2.10312720849350	3.15943106958926	-2.18271955813203
O	5.47651985016941	-2.27594892267700	-0.23016744591973
H	-1.98986057964113	-0.02793520930455	0.34868436836291
H	0.12574731711175	-0.69816752903969	0.07082455277097

S1.7) Tercer estado triplete optimizado, T₃

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Coordinates from ORCA-job opt

C	-5.07686705618666	0.94752428310401	0.38504511455589
C	-4.41227948636772	2.12828839007066	0.70024527291522
N	-2.85949356088147	0.50718858796942	0.40739945897824
C	1.47869636822130	3.18594084297527	-0.11024806546159
H	-0.80189749901760	5.40838796626867	1.45728081698342
C	-3.00432894718618	1.84056268516089	0.69852377519345
H	-4.31526658705028	4.09366414570499	1.57544677399535
H	-5.26147826105683	4.00876659710019	0.07703298097188
C	-4.07060817491755	-0.07023730629865	0.21965978608438
C	1.29118220436267	3.59951468510103	-1.58565873839697
H	0.81132123665342	3.62884323318328	1.85633709385319
C	-1.25134213353085	-3.29458610258374	-0.09406814273209
H	-1.35495090536032	-0.22607433948715	-3.80935771221744
C	-4.24455349345872	-1.44696310853613	-0.07008750848503
C	6.41897040824700	-0.62771368388466	1.58706676428811
C	4.58527511404861	1.95556267516863	0.69948456085860
C	-3.21275340259340	-2.35797539324376	-0.13834759639301
O	0.67441615866352	1.01186895350278	-2.84942255977865
H	-2.90177718082170	0.01008511480421	-2.91659127331987
N	-1.87876973448893	-2.09139756167449	-0.00780500854173
C	-2.23601475405139	-4.40001384294257	-0.29388148718317
H	-5.32690426696967	-3.98368605176430	-1.36927472986075
C	-3.44935964216862	-3.81434339483619	-0.33625618605080
H	-4.72634052076615	-5.51132907896730	-0.67840282701426
H	3.63726434095252	2.15903162980419	-1.14880471587473
C	-4.79593622791821	-4.42819418586553	-0.51283001818496
H	-5.42701992406804	-4.26105996606937	0.37447445260160
H	0.44180045055899	-4.56217552549307	-0.10835873129257
C	-1.89160255856732	-5.85308884851760	-0.37840803561037
H	-2.54088823243703	-6.42257434056109	1.62300190506626
H	-1.37811021627660	-7.55402362406820	0.88739748428563
H	-0.82177757100214	-5.98750735323198	1.52317084828321
O	5.75376836200177	2.23128274563422	0.57087691801618
C	-1.64257634370616	-6.49111377139807	0.99137204072684
H	-2.70840343971508	-6.38828518935274	-0.88532414122427
H	-0.99978193868325	-5.98443262835192	-1.01142894287496
C	-6.50333214801619	0.68015508474486	0.24912713499129
H	-6.78807977997893	-0.37348243339147	0.33280435411231
H	-5.26253249984199	-1.80521209737178	-0.20272559917927
C	-7.47897435377761	1.57049625059599	0.02670605363879
C	3.74096987419383	1.35710806870284	-0.40326942084037
H	-0.90716676669805	3.57991515355256	-1.67340012235870
C	-5.00518994452224	3.46298554017911	1.00009699527644
H	-5.93373283873177	3.35462064048080	1.57878222809756
H	-0.09503854221854	3.75800737453205	-3.21851545729076
C	-1.96196932108431	2.75741234091329	0.90525395419947
H	0.72033533487487	5.82183141001018	0.65201694331166
H	-8.51774056644389	1.24097351438953	-0.04833743528216
C	-0.60626457584754	2.55750271005260	0.73470708376626
C	-0.21617148358943	1.77541665325938	-2.56164066398679
H	-7.28753994396557	2.63601096581116	-0.10706710499761

C	0.10761299729823	-3.52945039746851	-0.03834472084219
C	2.38618439803280	0.80411192772272	-0.04016145825354
C	4.60911230283999	2.82810831549612	2.87901788179219
C	3.21075463986339	-1.64758824937925	0.13547860636438
O	3.89894389180093	2.21210863788047	1.81042435773022
C	1.13970880418865	-2.57019358737180	0.05578995586373
H	5.41388481711492	2.17143761960507	3.23723541050413
H	5.04569459771361	3.78243521419187	2.55387629067203
N	0.03376169290555	1.39091758728918	0.41741195141030
C	1.31388431413382	1.69363196014045	0.09206941521549
C	-1.80949406469233	0.06819873858588	-2.85370334953948
C	0.38248513416036	3.69883008100002	0.84033333157470
H	4.36717785006268	0.61163107691483	-0.90727323893871
H	-2.27555844101374	3.76936463643620	1.15169384431843
H	1.42160427410841	4.68946773190950	-1.64514363238037
H	-0.66382089509893	5.24576160846250	-0.30504815000348
N	1.00516007134958	-1.21567248637076	0.09351633603899
C	-0.12380016724174	5.11673474441176	0.64279262072566
C	2.54186616406890	-2.86386248870306	0.08374193433396
H	2.66108562900342	-4.83504509626488	0.92276676793551
H	2.85538605048775	-4.77288158527339	-0.83461479755673
H	2.46432615397248	3.53690828218736	0.21106415622935
C	2.22951143242959	-0.59196577064616	0.10251017779891
C	-0.03708278810820	3.23913504230244	-2.24669338232335
H	-1.45344069457616	-0.59661930631961	-2.05459582305884
C	4.67213207603886	-1.56978163086566	0.33331740978385
H	6.51256431885233	0.07542432115741	2.42026797460223
C	3.09843012305098	-4.24646950773675	0.10206052976799
H	4.18806289660255	-4.23693534499221	0.20781852681771
H	3.87751947286629	2.99641816696499	3.67664869645502
H	6.79109806920794	-1.61945644773622	1.87596386816915
H	6.98648066097886	-0.26046387751886	0.72244476527965
O	-1.50116689303142	1.42541200440645	-2.54534592906480
O	5.02693028568161	-0.69433774387114	1.27906918487749
H	2.10312720849350	3.15943106958926	-2.18271955813203
O	5.47651985016941	-2.27594892267700	-0.23016744591973
H	-1.98986057964113	-0.02793520930455	0.34868436836291
H	0.12574731711175	-0.69816752903969	0.07082455277097

S1.8) Cuarto estado triplete optimizado, T₄

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Coordinates from ORCA-job opt

C	-5.07686705618666	0.94752428310401	0.38504511455589
C	-4.41227948636772	2.12828839007066	0.70024527291522
N	-2.85949356088147	0.50718858796942	0.40739945897824
C	1.47869636822130	3.18594084297527	-0.11024806546159
H	-0.80189749901760	5.40838796626867	1.45728081698342
C	-3.00432894718618	1.84056268516089	0.69852377519345
H	-4.31526658705028	4.09366414570499	1.57544677399535
H	-5.26147826105683	4.00876659710019	0.07703298097188
C	-4.07060817491755	-0.07023730629865	0.21965978608438
C	1.29118220436267	3.59951468510103	-1.58565873839697
H	0.81132123665342	3.62884323318328	1.85633709385319
C	-1.25134213353085	-3.29458610258374	-0.09406814273209
H	-1.35495090536032	-0.22607433948715	-3.80935771221744
C	-4.24455349345872	-1.44696310853613	-0.07008750848503
C	6.41897040824700	-0.62771368388466	1.58706676428811
C	4.58527511404861	1.95556267516863	0.69948456085860
C	-3.21275340259340	-2.35797539324376	-0.13834759639301
O	0.67441615866352	1.01186895350278	-2.84942255977865
H	-2.90177718082170	0.01008511480421	-2.91659127331987
N	-1.87876973448893	-2.09139756167449	-0.00780500854173
C	-2.23601475405139	-4.40001384294257	-0.29388148718317
H	-5.32690426696967	-3.98368605176430	-1.36927472986075
C	-3.44935964216862	-3.81434339483619	-0.33625618605080
H	-4.72634052076615	-5.51132907896730	-0.67840282701426
H	3.63726434095252	2.15903162980419	-1.14880471587473
C	-4.79593622791821	-4.42819418586553	-0.51283001818496
H	-5.42701992406804	-4.26105996606937	0.37447445260160

H	0.44180045055899	-4.56217552549307	-0.10835873129257
C	-1.89160255856732	-5.85308884851760	-0.37840803561037
H	-2.54088823243703	-6.42257434056109	1.62300190506626
H	-1.37811021627660	-7.55402362406820	0.88739748428563
H	-0.82177757100214	-5.98750735323198	1.52317084828321
O	5.75376836200177	2.23128274563422	0.57087691801618
C	-1.64257634370616	-6.49111377139807	0.99137204072684
H	-2.70840343971508	-6.38828518935274	-0.88532414122427
H	-0.99978193868325	-5.98443262835192	-1.01142894287496
C	-6.50333214801619	0.68015508474486	0.24912713499129
H	-6.78807977997893	-0.37348243339147	0.33280435411231
H	-5.26253249984199	-1.80521209737178	-0.20272559917927
C	-7.47897435377761	1.57049625059599	0.02670605363879
C	3.74096987419383	1.35710806870284	-0.40326942084037
H	-0.90716676669805	3.57991515355256	-1.67340012235870
C	-5.00518994452224	3.46298554017911	1.00009699527644
H	-5.93373283873177	3.35462064048080	1.57878222809756
H	-0.09503854221854	3.75800737453205	-3.21851545729076
C	-1.96196932108431	2.75741234091329	0.90525395419947
H	0.72033533487487	5.82183141001018	0.65201694331166
H	-8.51774056644389	1.24097351438953	-0.04833743528216
C	-0.60626457584754	2.55750271005260	0.73470708376626
C	-0.21617148358943	1.77541665325938	-2.56164066398679
H	-7.28753994396557	2.63601096581116	-0.10706710499761
C	0.10761299729823	-3.52945039746851	-0.03834472084219
C	2.38618439803280	0.80411192772272	-0.04016145825354
C	4.60911230283999	2.82810831549612	2.87901788179219
C	3.21075463986339	-1.64758824937925	0.13547860636438
O	3.89894389180093	2.21210863788047	1.81042435773022
C	1.13970880418865	-2.57019358737180	0.05578995586373
H	5.41388481711492	2.17143761960507	3.23723541050413
H	5.04569459771361	3.78243521419187	2.55387629067203
N	0.03376169290555	1.39091758728918	0.41741195141030
C	1.31388431413382	1.69363196014045	0.09206941521549
C	-1.80949406469233	0.06819873858588	-2.85370334953948
C	0.38248513416036	3.69883008100002	0.84033333157470
H	4.36717785006268	0.61163107691483	-0.90727323893871
H	-2.27555844101374	3.76936463643620	1.15169384431843
H	1.42160427410841	4.68946773190950	-1.64514363238037
H	-0.66382089509893	5.24576160846250	-0.30504815000348
N	1.00516007134958	-1.21567248637076	0.09351633603899
C	-0.12380016724174	5.11673474441176	0.64279262072566
C	2.54186616406890	-2.86386248870306	0.08374193433396
H	2.66108562900342	-4.83504509626488	0.92276676793551
H	2.85538605048775	-4.77288158527339	-0.83461479755673
H	2.46432615397248	3.53690828218736	0.21106415622935
C	2.22951143242959	-0.59196577064616	0.10251017779891
C	-0.03708278810820	3.23913504230244	-2.24669338232335
H	-1.45344069457616	-0.59661930631961	-2.05459582305884
C	4.67213207603886	-1.56978163086566	0.33331740978385
H	6.51256431885233	0.07542432115741	2.42026797460223
C	3.09843012305098	-4.24646950773675	0.10206052976799
H	4.18806289660255	-4.23693534499221	0.20781852681771
H	3.87751947286629	2.99641816696499	3.67664869645502
H	6.79109806920794	-1.61945644773622	1.87596386816915
H	6.98648066097886	-0.26046387751886	0.72244476527965
O	-1.50116689303142	1.42541200440645	-2.54534592906480
O	5.02693028568161	-0.69433774387114	1.27906918487749
H	2.10312720849350	3.15943106958926	-2.18271955813203
O	5.47651985016941	-2.27594892267700	-0.23016744591973
H	-1.98986057964113	-0.02793520930455	0.34868436836291
H	0.12574731711175	-0.69816752903969	0.07082455277097

S2. Zinc trimetil éster de clorina e6 (ZnTMEe6):

S2.1) Estado basal optimizado, S₀

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Coordinates from ORCA-job opt

C	5.18767732511786	-0.67946511160752	0.45612963126740
C	4.66396292297594	-1.92137826057552	0.69875428540035
N	2.87779204698215	-0.48898794356959	0.39652676870724
C	-1.12547482121117	-3.44933804690714	-0.34992928494035
H	1.43270899528614	-5.65165883239955	0.74266265824245
C	3.21159848010497	-1.77337001333768	0.63280198183679
H	6.35820261491729	-3.00338354392718	1.44980094293456
H	4.79426398830130	-3.81328305622200	1.71115637657993
C	4.04989564178319	0.22636359876600	0.27959116936115
C	-0.96379444264081	-3.60499536238204	-1.87756281822640
H	-0.34380610307971	-4.16783461865411	1.49707947649617
C	1.02940735321969	3.30894396124498	0.01765826012395
H	-0.05678500086128	1.02302369773260	-4.04975303674516
C	4.13530752160467	1.57544111957452	0.04317766673779
Zn	0.98581351920639	0.24400717649619	0.19234415541540
C	-4.25648674100865	-2.49370281029369	0.59036369689517
C	3.05513530090449	2.48547007131987	-0.04692982338056
O	-1.54797647816344	-1.08808240703224	-3.33356045268068
H	0.82205314625195	1.65165403025393	-2.60585341946557
N	1.75008813904966	2.14175943528723	0.03174629084127
C	1.92195579377481	4.43710088291543	-0.10729205462540
H	5.10832593935594	4.50703613675629	0.66023340813904
C	3.19664650016947	3.91794806422387	-0.14918508311746
H	5.09767762999136	4.30624374642796	-1.09841476051863
H	-3.32402696226212	-2.39054521670455	-1.28211151986949
C	4.49564728248204	4.65236676768692	-0.24374398918816
H	4.33416529343940	5.73196105492314	-0.36348550996319
H	-0.78257127985085	4.37937057981830	0.17265821331678
C	1.51378822420656	5.87901406214639	-0.10571395390265
H	1.08543701203350	7.52078686322343	1.26945457002863
H	0.63603526271764	5.91367313570417	1.89182712808288
H	2.34402757318974	6.39779534787100	1.84262673676732
O	-3.78373489079914	-3.05147595843101	1.54999049813774
C	1.38679306186209	6.46297790142238	1.30386918149669
H	2.25024501040986	6.46471937100247	-0.67675475274131
H	0.55680323324276	5.99585363520712	-0.63740793203746
C	6.58499926220551	-0.25494738882849	0.39457384592261
H	6.77958333238847	0.78596277175433	0.67298244305894
H	5.13365494265990	2.00540834828465	-0.03909490323852
C	7.62398751223501	-1.01008394368491	0.02090113398107
C	-3.48591987256309	-1.70279394571999	-0.43917871955267
H	1.00819385251754	-2.61481216274502	-1.99185063091600
C	5.37191775941638	-3.19809197669079	1.00708857455234
H	5.53441206251610	-3.80505697622590	0.10114189968683
H	0.31352449516265	-3.10019703456869	-3.53732688826997
C	2.30847131098781	-2.84013234594896	0.73734392066100
H	-0.04502119295825	-6.07308557067295	-0.13993268355404
H	8.63653019195057	-0.59962684239269	0.01543151463956
C	0.93689472780760	-2.77571173363276	0.56449311196415
C	-0.47272333133729	-1.30678175633288	-2.83115446546739
H	7.50473044654594	-2.04376968919890	-0.31011105274181
C	-0.35235270485326	3.37771230693856	0.15966532360402
C	-2.16136710727492	-1.13529117133947	0.01666307859468
C	-6.38691697813469	-3.28534798315059	1.16419987283855
C	-3.18181925279042	1.18957357463517	0.48674768443230
O	-5.54580198642741	-2.57923111564862	0.26134043189391
C	-1.25340325445960	2.32507558062606	0.28984676323924
H	-6.02989126644631	-4.31420961886259	1.31051032404859
H	-6.41231599948332	-2.77404503929546	2.13702658154062
N	0.20422394976722	-1.65676585252278	0.40255098190440
C	-1.08493224000362	-1.98516903493455	0.05493990133543
C	0.02357919594619	0.98880111766451	-2.95490239484590
C	0.05088882221096	-4.00065234171565	0.47826239463900
H	-4.14359085417609	-0.92827654542787	-0.84705671749529
H	2.73798171738358	-3.82928753983328	0.88414636911144
H	-0.71225985242736	-4.65103677549671	-2.09744656034713
H	1.24427576699580	-5.14524792735807	-0.94792747485449
N	-0.93191276552344	0.98297560059124	0.21049822584630
C	0.70840788207953	-5.28434993852210	0.00183965767558

C	-2.66748652546023	2.47676025116493	0.46600485956289
H	-4.00401509731172	3.99335693438912	-0.25627979934915
H	-4.10453674044565	3.71246716213676	1.48000959990035
H	-2.05774222703661	-3.93614209701486	-0.04732945141909
C	-2.07675002337037	0.27749774727216	0.28171425110077
C	0.06572395083045	-2.68713317423449	-2.54592927536913
H	-0.93283404537537	1.28304389910106	-2.50665431069507
C	-4.54798245261101	0.83897891605880	0.89968489908987
H	-6.87217987060520	1.51874257436522	1.99385087391018
C	-3.40249259471863	3.76595026461988	0.63665669830929
H	-2.71881756520812	4.60547065753444	0.81254157261580
H	-7.38674799599908	-3.29103615664283	0.71628874387624
H	-7.40307750338673	2.29139368470758	0.45667521405323
H	-7.15567919234451	0.50958278130726	0.54657496380107
O	0.39143932997991	-0.32703576040647	-2.53189490365909
O	-5.46171995857599	1.71491491483260	0.47269419074065
H	-1.93127507936918	-3.42272566603274	-2.36690073830683
O	-4.84314121795533	-0.11201124177978	1.59118966768786
C	-6.80203985565801	1.48884680091711	0.89759669485660

S2.2) Primer estado single optimizado, S₁

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Coordinates from ORCA-job opt

C	5.18334261571769	-0.68944862027704	0.41535075140265
C	4.65537872933787	-1.95070600491925	0.65835820452014
N	2.88852994080278	-0.49729307954560	0.36124294526841
C	-1.13480626318815	-3.42960691888184	-0.36499811892454
H	1.37381184660745	-5.66175649744157	0.78343749342402
C	3.22473930985010	-1.80524945229775	0.60389879432299
H	6.21483423774798	-3.05341009689714	1.64284374209435
H	4.72739077242569	-3.98450267272146	1.36910553193662
C	4.04604628703511	0.19926713931374	0.24130233895204
C	-0.94274436944817	-3.58521711876084	-1.89030807045324
H	-0.38918365457945	-4.13994167398384	1.49618146925540
C	1.03058463486332	3.29201363526923	0.02741983632578
H	0.03389703983848	1.03066024581952	-4.04171834830007
C	4.12557919032426	1.59112024008157	-0.00054642769797
Zn	0.98734050560243	0.23649444287036	0.17745968475395
C	-4.26954511057466	-2.48882451688061	0.56391087600704
C	3.06446262799310	2.46679624804942	-0.07363715650940
O	-1.47475499482424	-1.07577214618786	-3.37709239527817
H	0.86607122849873	1.66551316577263	-2.57284821317464
N	1.73813375809933	2.13002967329562	0.03179845323026
C	1.93643344142873	4.43641797106744	-0.12923875241766
H	5.12368074063701	4.49549821768612	0.55383683810663
C	3.19431286220504	3.92481269320928	-0.19968848775679
H	5.06710108983991	4.26983011867073	-1.19982013006194
H	-3.33888035439504	-2.36131889821228	-1.30890884135636
C	4.49331240134803	4.64325997418808	-0.33741598357771
H	4.34261062099487	5.72260766253383	-0.46801021413282
H	-0.77153277791003	4.39247077875338	0.18753311028448
C	1.50914368490385	5.87086562490220	-0.13557128901191
H	0.97495385453668	7.49063888815388	1.22531641463618
H	0.53085600975361	5.87206998100394	1.81832117532072
H	2.22868059415540	6.39240481734155	1.85492916708191
O	-3.79234077696853	-3.06179053097072	1.51257377119306
C	1.29779892583038	6.43984509397908	1.27036688856327
H	2.26695516804180	6.47067021631921	-0.66121377735042
H	0.57958311897355	5.97541910868273	-0.71706963971399
C	6.56892537183711	-0.25250561540351	0.35289604900897
H	6.71885219380990	0.83101035923328	0.39218852748400
H	5.12091971837198	2.02237543285987	-0.09659803156908
C	7.66980429305120	-1.01322727514041	0.24906250593835
C	-3.50008558305241	-1.68440040420981	-0.45631974771170
H	1.03875518245868	-2.60943646040350	-1.96224719318020
C	5.38744840627882	-3.22124675920393	0.93651506634559
H	5.83270536927508	-3.64996104763527	0.02270739844195
H	0.37338627753045	-3.09369967904585	-3.52161585507486
C	2.29589014128885	-2.85683664580310	0.71127791927781

H	-0.10177070606877	-6.06541464952972	-0.11132739076352
H	8.65787179234775	-0.54805312617243	0.21975557324699
C	0.92397729816032	-2.77804789801312	0.56060972259214
C	-0.41830918903515	-1.29432029729737	-2.83698096517409
H	7.63406745709726	-2.10054217463580	0.17499620299613
C	-0.35000173376956	3.38876185250462	0.17394548603001
C	-2.17758797051392	-1.12269967688595	0.00747785890703
C	-6.39881008821765	-3.28715071119390	1.13283617750006
C	-3.19021922715453	1.19712188189926	0.52568017444670
O	-5.55955185899488	-2.56929209947233	0.23746277040206
C	-1.25387098831828	2.32650653556287	0.30734314710392
H	-6.03550196431611	-4.31445589365214	1.27399666223361
H	-6.43080884788625	-2.78176231989551	2.10863346591990
N	0.19236629494867	-1.64277527986318	0.40063342284632
C	-1.09251502176632	-1.97153341829345	0.04251893509732
C	0.07897220668647	1.00190494956200	-2.94483868673606
C	0.02612356099934	-3.98981114369469	0.48261516494028
H	-4.15778167928068	-0.90374930812740	-0.85297912348992
H	2.70812322119005	-3.85338293746547	0.85815412045451
H	-0.69651569807634	-4.63367567627568	-2.10404482123117
H	1.21478616610403	-5.17358754377416	-0.91603299580618
N	-0.93495291903756	0.99127283675312	0.21632881933811
C	0.66587923367152	-5.29021834054294	0.02919487093251
C	-2.67233456739102	2.48211291043229	0.50764375999026
H	-3.91374540254266	4.07734679054501	-0.22100197725279
H	-4.15144186976723	3.69871849511273	1.48345091615009
H	-2.07745876521383	-3.90827513857555	-0.08303665801421
C	-2.08607964456348	0.28134124886962	0.29552995296983
C	0.10795998924883	-2.67630170013076	-2.53676001154513
H	-0.89161841512550	1.29839998318792	-2.52925556868748
C	-4.54824563848622	0.83641398200397	0.94788143109316
H	-6.85847174779697	1.47419425548516	2.09786646458353
C	-3.38673416780150	3.77770083010439	0.69937948991156
H	-2.69508803808441	4.58535921357256	0.97051122160728
H	-7.39726156078207	-3.29648105126532	0.68188926893785
H	-7.40826870119346	2.30554360617946	0.59847850614268
H	-7.16052408093545	0.52168318521341	0.61641091648806
O	0.43280870912595	-0.31287815845346	-2.50436778531869
O	-5.46723610669836	1.72918944641604	0.56732669035481
H	-1.89981661252349	-3.39359011326762	-2.39610249287759
O	-4.83549232633548	-0.13981321999739	1.60821280582875
C	-6.80182669825763	1.48673925883736	1.00045619792830

S2.3) Segundo estado single optimizado, S₂

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Coordinates from ORCA-job opt

C	5.13235253465516	-0.69643241943760	0.46119318742889
C	4.59313879019809	-1.95531283480670	0.72996362738342
N	2.84253731804293	-0.52880122362004	0.30434441260953
C	-1.14449854457702	-3.43432616035985	-0.45205882183554
H	1.31144037389228	-5.68929157645913	0.75822381100080
C	3.17571091649820	-1.81082846339661	0.61601075420929
H	6.08237869414417	-3.01828577979658	1.85864610541443
H	4.63880149384949	-3.97791161879348	1.47982900148685
C	4.00979837547715	0.17736058536566	0.21410166895695
C	-0.87094179598933	-3.51796240750569	-1.96958231149707
H	-0.49674016307552	-4.18843313261687	1.42799804657790
C	0.98220954053718	3.28455148834615	-0.03986974951494
H	0.26080298537720	1.05320707106121	-4.01408529520593
C	4.08085831754979	1.55539634863601	-0.05103172869938
Zn	0.94661715964035	0.23117198904853	0.08332028159325
C	-4.28272941894255	-2.54290557434455	0.44666135446236
C	3.01269287379053	2.44530225323790	-0.13253406767166
O	-1.32267721785753	-0.91323695548000	-3.31324661346226
H	1.18230462194687	1.70825949593856	-2.60898968371568
N	1.69824806741394	2.11433343063955	0.01067562013207
C	1.88800234458112	4.40807036877648	-0.24474451766289
H	5.08613258635291	4.49835342705763	0.40742956659567
C	3.15013651047310	3.88382436876618	-0.30774110176221

H	5.01928524224752	4.19524972304754	-1.33474430365981
H	-3.33405065477278	-2.32869382057191	-1.41340896895526
C	4.44821577631977	4.60017687391949	-0.48493099873368
H	4.29165787567682	5.67224497665861	-0.66220955946676
H	-0.80403605227642	4.38605358594270	0.11340801955283
C	1.47905580285132	5.84738969917375	-0.29931917772173
H	1.01870543107771	7.53163883916342	1.01075556199118
H	0.56963373049333	5.94496013927602	1.68306609015781
H	2.27541783640242	6.43833033210006	1.64269057499605
O	-3.80132715250172	-3.15225789723454	1.36922945086687
C	1.32612962324377	6.47796120106610	1.08772766394691
H	2.22499370450359	6.41410822258284	-0.87655622954433
H	0.53068289506288	5.94204555147181	-0.85085356130697
C	6.52165166529475	-0.26186547801071	0.44439751468042
H	6.66920093869201	0.82246335949805	0.42483885764493
H	5.07555409316093	1.98817034790559	-0.15579456362708
C	7.62681836314175	-1.02211719951939	0.44356627398073
C	-3.51913008468843	-1.68546587144966	-0.53895579244753
H	1.12103740573816	-2.55774370691598	-1.90552297250795
C	5.31925520776626	-3.21020960518860	1.08908546259874
H	5.84425506379371	-3.64429192873235	0.22206575763394
H	0.51920418101754	-2.94528895363943	-3.51202424541668
C	2.22900304338434	-2.86577583768709	0.73210727772256
H	-0.12919173381872	-6.08193055881277	-0.19633234112385
H	8.61401163013267	-0.55437924909512	0.43336435447738
C	0.86553403087332	-2.80362687567571	0.57912404420471
C	-0.28057315817722	-1.18156231572935	-2.77291009782195
H	7.59794367368354	-2.11196144825070	0.43876609180115
C	-0.38534601126074	3.37979982117520	0.10849378217573
C	-2.21445775040627	-1.12792992027997	-0.03888951531348
C	-6.40954323910734	-3.36888619824689	0.97633513552469
C	-3.22023666119856	1.17156188925081	0.58721481907713
O	-5.56843000725560	-2.61628242712522	0.11086376378226
C	-1.31363252871775	2.31940623909278	0.26645750619211
H	-6.04272787139623	-4.39908928563599	1.08223559013139
H	-6.44744299914955	-2.89755862673618	1.96871471315707
N	0.12181375880618	-1.66633306055798	0.44014099756597
C	-1.12680184292228	-1.98971738206861	0.01478744367593
C	0.33486000939242	1.09016317346644	-2.91985357931010
C	-0.03061654686882	-4.01637077827581	0.44027923258614
H	-4.18478004044598	-0.89417040684413	-0.89727053132651
H	2.64698146834678	-3.86103957962350	0.87991789761874
H	-0.61133148496419	-4.55506042372693	-2.22100630974444
H	1.21152056208433	-5.17005638055889	-0.93636440762077
N	-0.99842328742680	0.98817656752048	0.12203938929189
C	0.62889440219815	-5.30607550820423	-0.01383521222261
C	-2.69460616566386	2.47208946544645	0.55549631114239
H	-4.13658124010432	3.98617878816645	0.03786661889448
H	-3.95882012175752	3.72148520285826	1.76876005374272
H	-2.09475187435815	-3.93300144906563	-0.24081144450536
C	-2.14269087745561	0.27655759428482	0.27834110525699
C	0.21286321843312	-2.58236461643953	-2.51692278736586
H	-0.59741028218898	1.48345677813637	-2.49767345884989
C	-4.54901432731031	0.79553993524432	1.06933630021409
H	-6.71906457761164	1.30536690439250	2.51566100182655
C	-3.39931879574934	3.76243422961962	0.82352392448235
H	-2.69569874292721	4.60231081065432	0.88161990151092
H	-7.40542115479306	-3.36524065794926	0.51987969978112
H	-7.34449116441289	2.41739967176701	1.24615363713565
H	-7.20494216044628	0.65155342515636	0.92598047089590
O	0.60021663776942	-0.22544723343228	-2.40905182017291
O	-5.45236390210175	1.77377632970223	0.92907093685159
H	-1.79934188964154	-3.30110455989308	-2.51757878973594
O	-4.83816543285663	-0.26689060918808	1.58324199535924
C	-6.75473981883247	1.51407649236835	1.43716189754836

S2.4) Tercer estado single optimizado, S₃

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Coordinates from ORCA-job opt

C	5.17359968351075	-0.70783284801601	0.43820048283142
C	4.64100948291531	-1.95471754577304	0.67970303202184
N	2.86432063989498	-0.50363774405045	0.37928089938593
C	-1.14439060563957	-3.42532384627980	-0.38388807962322
H	1.37506454053018	-5.67077261080601	0.71263397809086
C	3.20055346385880	-1.80273652507577	0.62042221628602
H	6.28602299809552	-3.04096413052846	1.52622143035048
H	4.73471024327375	-3.91046314201422	1.57540185516121
C	4.03532462719493	0.20234065567658	0.26296363015697
C	-0.94982687688420	-3.53851152158189	-1.91353245984015
H	-0.39993582404039	-4.17839827533552	1.46140757948922
C	1.02271977182648	3.31182358778513	0.05367383152540
H	0.12692356533746	1.07659294127725	-3.99065476878515
C	4.12470453682169	1.56304093338980	0.02135827444304
Zn	0.97792055153623	0.24776071333262	0.19883065075651
C	-4.26411497274794	-2.49005650584122	0.62512166846289
C	3.04943627708977	2.48185087886384	-0.04759977447815
O	-1.44560862825774	-0.95936846352954	-3.28552015658688
H	1.02785724291196	1.68521223569002	-2.55174091008551
N	1.73370872752881	2.14637343454752	0.08782023127999
C	1.90590676010968	4.43128644869945	-0.13216518927512
H	5.11875583648566	4.54117289775292	0.53529979201935
C	3.18846131579039	3.90514094425321	-0.19849746840554
H	5.07063207033551	4.23801779108138	-1.20653561580873
H	-3.36692669421410	-2.37021586870882	-1.26582585953438
C	4.48274419175223	4.63201789640572	-0.36156115535561
H	4.31776543439487	5.70326368422610	-0.54044574468498
H	-0.81769568565396	4.38171274514137	0.23471476492856
C	1.49314628288775	5.86971514596022	-0.17679301721540
H	1.04570403903158	7.55866619006314	1.13707630522500
H	0.59958775098929	5.97211717934074	1.81260416169388
H	2.30570430752492	6.46226587296489	1.75849583941548
O	-3.76255366976484	-3.05405922530687	1.56597206821722
C	1.35221754553509	6.50385980869253	1.21064681117300
H	2.23077994724768	6.44109851128175	-0.76170885418701
H	0.53779298737737	5.96679161001378	-0.71768588206081
C	6.56424808136309	-0.28223738308024	0.38608315210231
H	6.73885060056433	0.78060469489555	0.58483710623157
H	5.12389413420757	1.98517195753463	-0.08673738742663
C	7.63295895610087	-1.04535805058394	0.11500561228686
C	-3.52012345440320	-1.68736553450451	-0.41647893524599
H	1.04758573555618	-2.59315361287030	-1.95209593935407
C	5.35466655476259	-3.23174560555645	0.97396653885742
H	5.63155908310044	-3.76983997020632	0.05185693014394
H	0.37575853368012	-3.00916011746301	-3.52580730948391
C	2.28189703877148	-2.85794577189433	0.72349767365526
H	-0.09794173174156	-6.06357712344425	-0.19080899981330
H	8.63672237784890	-0.61409808339802	0.11902822459490
C	0.90723111626671	-2.78611071539093	0.56376794910239
C	-0.38259357801331	-1.22209609705851	-2.77989851088565
H	7.54917627274761	-2.10399729280245	-0.13656033766629
C	-0.38033389353867	3.38351215680908	0.20834767431492
C	-2.19489209587921	-1.11501027351557	0.02212797835390
C	-6.37855470061518	-3.28582351770384	1.24982577564889
C	-3.21132169091034	1.19750453133952	0.52563752725931
O	-5.56110153406916	-2.57013359471640	0.33146756635711
C	-1.26347890241584	2.32068248774167	0.32800852172718
H	-6.01125013334302	-4.31258279128058	1.38365884441637
H	-6.38567948188962	-2.77763145935521	2.22452085220153
N	0.16953625543106	-1.65549973880420	0.42790879566059
C	-1.10219368644796	-1.97505219892949	0.05248367225454
C	0.20155568651246	1.05510657153574	-2.89534229870671
C	0.01616330492493	-4.00108537080413	0.45150013840299
H	-4.18964636414373	-0.91496847004185	-0.80945982327365
H	2.70115857433427	-3.85325300810057	0.86084931113158
H	-0.71535935162392	-4.58327144965987	-2.15792494483834
H	1.21211163155646	-5.14418888856459	-0.97510287515289
N	-0.94535094966717	0.98520219794732	0.23276223287035
C	0.66425775865695	-5.28643613330215	-0.03259081932215

C	-2.69487651434651	2.47305536184145	0.52437352163047
H	-3.27697358863748	4.41696389432532	-0.15647956997354
H	-4.43350362609488	3.66044337503431	0.96057994727280
H	-2.08559867376551	-3.91545150537805	-0.11617262513044
C	-2.10606530227310	0.27666082934699	0.30188101423989
C	0.11489360159749	-2.62338562462011	-2.52659287900720
H	-0.74274857542613	1.39751200229735	-2.45548637593234
C	-4.57465823188046	0.81982646997171	0.93926770639402
H	-6.96233079327274	1.42416972983493	1.93455848351629
C	-3.36822553785360	3.78349254266749	0.74125104863882
H	-2.89259733219375	4.33615123132978	1.56653795851364
H	-7.38753728689806	-3.29573232387832	0.82330705322749
H	-7.48964701652107	2.08287226429613	0.34340498015794
H	-7.14582590764527	0.32520269047574	0.53601625385246
O	0.50944816736226	-0.27203552204051	-2.45383974131244
O	-5.52022835653996	1.61860389551703	0.44167525483104
H	-1.90266056565079	-3.31853133798147	-2.41609878020818
O	-4.83149183851675	-0.10273473163228	1.68131152472268
C	-6.85943263371376	1.34012956022832	0.84393676117468

S2.5) Primer estado triplete optimizado, T₁

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Coordinates from ORCA-job opt

C	5.13608198180003	-0.69148183074563	0.45410269879440
C	4.60806735877573	-1.94269283674453	0.75356123764213
N	2.84868844326251	-0.50944214961053	0.35016635943582
C	-1.13483122108289	-3.42933261445861	-0.41368499837225
H	1.33045674426490	-5.65557806914815	0.83621911388193
C	3.17615816560772	-1.80552130402056	0.66990373631653
H	6.15910832887659	-2.98313870342712	1.81246212548407
H	4.67595416353949	-3.93364847254916	1.57466429720752
C	4.00489292843976	0.17306090493857	0.21725000740808
C	-0.85307543640802	-3.55003494533939	-1.92661654618997
H	-0.47425324553254	-4.15039516248546	1.48098972623452
C	1.00087950156614	3.26944700474244	-0.03406415813282
H	0.22653054212617	1.00896192197265	-4.03071968428947
C	4.08291826800427	1.57341848808196	-0.09108055150793
Zn	0.94808622432271	0.21821182940136	0.09629520315586
C	-4.33970457558492	-2.52029251787285	0.35083246013527
C	3.03489045520963	2.44475657412620	-0.17434348156146
O	-1.29228764526764	-0.99758374108504	-3.37668994319601
H	1.13286654792722	1.67933780744021	-2.62306729351133
N	1.69920998811992	2.11470873064987	-0.02145636192846
C	1.90338359336289	4.41100122302254	-0.24712313753792
H	5.10389640467706	4.50838323584309	0.33360611910504
C	3.15804006101783	3.89834920717759	-0.34644835562781
H	5.00344685143362	4.20896228244823	-1.40753498931583
H	-3.32027034225379	-2.28346978621913	-1.46160082327872
C	4.45032222581449	4.61535969532443	-0.54667659190237
H	4.29080876355402	5.68780995597192	-0.71812852520154
H	-0.78827925606196	4.38469958116267	0.19604183749241
C	1.47392002846748	5.84485041774634	-0.27828488660800
H	0.96654295863005	7.49708948608475	1.05308561824634
H	0.54251724216416	5.89371201971821	1.69874560574214
H	2.23881546250881	6.41933936213769	1.68053381033030
O	-3.91514427868996	-3.20910253334559	1.24594113333844
C	1.29407952582983	6.44870037716649	1.11735150321098
H	2.21811335562036	6.43278556106205	-0.83588256989041
H	0.53085417265713	5.93391318073060	-0.84046517500931
C	6.52588296353987	-0.25375484445794	0.39885922346513
H	6.67424022846498	0.83053326463610	0.41195232981550
H	5.08027788394699	1.99244876140105	-0.21917388159325
C	7.62591328751496	-1.01629377221406	0.33281839090151
C	-3.51211275756452	-1.65992396874492	-0.57437419017818
H	1.13859989806417	-2.58477615938136	-1.87934978021159
C	5.33938243475058	-3.19326460812063	1.10907257624999
H	5.79424119178999	-3.66724369528138	0.22328548208392
H	0.54416788387445	-3.02344998743867	-3.47718678118470
C	2.24778694719244	-2.84422221280710	0.81384523095174

H	-0.09468462758499	-6.05595223398427	-0.13835180226866
H	8.61481948217123	-0.55316836461356	0.30619454487172
C	0.86904718232877	-2.76501982567585	0.61690548742798
C	-0.26489457802764	-1.23914605877856	-2.79585463412858
H	7.58981801388927	-2.10514687431563	0.28784509395281
C	-0.37962068491449	3.37637817184101	0.15626197795877
C	-2.20383186011936	-1.14288719293638	-0.02288712545044
C	-6.51417917708229	-3.27205491379745	0.79488485677847
C	-3.19508261999071	1.17187472033395	0.63848497346271
O	-5.62451335629883	-2.50675334632697	-0.00709751853622
C	-1.28764105908317	2.32502502348248	0.31172732840576
H	-6.20771855259735	-4.32687224291396	0.82484158309485
H	-6.53501469522696	-2.87673825278890	1.82045863649787
N	0.15739352809742	-1.64511229537324	0.42830127575139
C	-1.13804057561650	-1.98023326912540	0.02535848772651
C	0.29961808285219	1.04329725002455	-2.93627277849424
C	-0.01473969730338	-3.98803624080986	0.48907650419997
H	-4.14377942480018	-0.84299749611655	-0.93984817501581
H	2.65266983656746	-3.83561485670863	1.00822631676714
H	-0.59577060507681	-4.59327789638710	-2.15324733092533
H	1.25381225169294	-5.14488218651107	-0.86242518114170
N	-0.97934512559901	0.98528000008046	0.15527330911046
C	0.65883855723270	-5.27768443420597	0.05243283851639
C	-2.68105512329222	2.46925876772482	0.61143273399211
H	-4.11364663833157	3.98207689583770	0.08976173495784
H	-3.96168214097382	3.69957646355520	1.82002773539956
H	-2.08449236318472	-3.92664156753178	-0.19491508751503
C	-2.11262419473500	0.28055482511011	0.30639293221904
C	0.23381500906651	-2.63028238157264	-2.49508319161362
H	-0.64123927283769	1.41669955354423	-2.51404277629201
C	-4.51889398619771	0.77921100018264	1.12388415299322
H	-6.69535152647267	1.25605583526126	2.57032154748381
C	-3.38745880409958	3.75478935810714	0.88480326562955
H	-2.68591334817294	4.59464585658018	0.96021958820517
H	-7.50444417002437	-3.17792553325622	0.33562777474778
H	-7.33619681688474	2.36148290867877	1.30247398754983
H	-7.17120056545566	0.59836001605376	0.97875822834623
O	0.59111677358684	-0.26557045936214	-2.42718605175423
O	-5.43490970357986	1.74472600723698	0.98468301856254
H	-1.77964050984422	-3.34368959435108	-2.48134380683502
O	-4.78776674536783	-0.28650502449713	1.63940918269932
C	-6.73416850798182	1.46614193081589	1.49231324226185

S2.6) Segundo estado triplete optimizado, T₂

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Coordinates from ORCA-job opt

C	5.10674531697866	-0.68158267369222	0.49000784695557
C	4.56191373775367	-1.95271228960712	0.75118392362586
N	2.82376528087930	-0.52287947461799	0.31391320199227
C	-1.15933191501937	-3.45112227445994	-0.50074689831023
H	1.30605426451638	-5.70923095804671	0.68702230916687
C	3.15831151025659	-1.80878953189448	0.62222318917496
H	5.85896506523371	-3.10277403073613	2.03362902838327
H	4.61938555543781	-4.06233671398568	1.21073589942282
C	3.99132412048324	0.17986330234211	0.22527184220422
C	-0.89541634605632	-3.52955544668465	-2.02077505807622
H	-0.50699222364189	-4.22148486256646	1.37098380518178
C	0.98513180501529	3.30033173126226	-0.08443636537475
H	0.22616562242129	1.05060155763834	-4.05280520203483
C	4.07250264252707	1.56248758135904	-0.05788935053155
Zn	0.94761222750629	0.23290847288989	0.07153159041612
C	-4.27445672050528	-2.54802109135517	0.43125786282039
C	3.01216352380211	2.45747254968503	-0.16524946489952
O	-1.35498806811833	-0.91091586423764	-3.32435356367233
H	1.19357579695104	1.68435708187538	-2.66927345588858
N	1.70260205633363	2.12821227144664	-0.03450914909835
C	1.89450731665400	4.42365444435790	-0.29271490396401
H	5.08313141573846	4.51555213494014	0.38136856128693
C	3.15300912482874	3.89876219982417	-0.34783130014164

H	5.03420046426413	4.19194627615474	-1.35774895026214
H	-3.35707115458752	-2.31065071936250	-1.44581502941224
C	4.45530299050982	4.60879495166246	-0.51908983192457
H	4.30415070766987	5.67925878886239	-0.71055721386425
H	-0.80340337056912	4.38560231196355	0.08257035626361
C	1.48417953409582	5.86248355900569	-0.35335917543440
H	1.02158199686100	7.55285385261108	0.94714895884620
H	0.57332566171498	5.97022196301822	1.62860254635629
H	2.27886341182413	6.46429807277132	1.58575964229203
O	-3.77608558456435	-3.16371325918636	1.34080252241991
C	1.32975557626902	6.49987128589238	1.03025279274418
H	2.23018874862971	6.42708257254064	-0.93258969773942
H	0.53605382761179	5.95327764007765	-0.90597746506140
C	6.49508158347008	-0.24828473749915	0.47592041030455
H	6.64846940220067	0.79796792988342	0.19495695331940
H	5.07040001674743	1.98884493788491	-0.15301787120109
C	7.59785593165179	-0.95848236615539	0.75868323317772
C	-3.52877104158348	-1.68170289613011	-0.55842646654184
H	1.10225342772251	-2.57950420705630	-1.97175290733618
C	5.29737398939402	-3.20789420972023	1.09170282988474
H	6.03023789632273	-3.47064024012079	0.31259957897252
H	0.48184361765878	-2.95504142256009	-3.57404668668901
C	2.20990862736189	-2.87847562521952	0.70545792846062
H	-0.13491458268826	-6.10144691341799	-0.26711925313352
H	8.58110060719642	-0.48675403953246	0.69904750449686
C	0.85539442788955	-2.82896502459790	0.53255003192733
C	-0.3000555550187	-1.18961466517645	-2.81393932545604
H	7.57271536996495	-2.00617665174478	1.05581280176224
C	-0.37365550257276	3.38413640537898	0.08198188211443
C	-2.21431266492140	-1.13719740602155	-0.06525920823592
C	-6.39325053440772	-3.36433593799821	1.00331086564884
C	-3.19457879851015	1.15601295616773	0.61541569786857
O	-5.56617268127875	-2.61599179648900	0.12059641368376
C	-1.29992294252179	2.30751482994182	0.26604570728210
H	-6.02915635626957	-4.39612402362492	1.10293611862193
H	-6.40859818984175	-2.89155398878302	1.99565747234640
N	0.11383221633270	-1.68555504740224	0.38665138089497
C	-1.13475331579687	-2.00734492893185	-0.02945417585324
C	0.33146967387776	1.07687011348478	-2.96068587144052
C	-0.04240078921089	-4.03942156336219	0.38468283193564
H	-4.19668354111690	-0.88270476099064	-0.89366288793840
H	2.63370577416851	-3.87236509538640	0.84800412592093
H	-0.64061137447480	-4.56692000090615	-2.27606724815242
H	1.20041764967967	-5.17805696281206	-1.00359595877087
N	-0.98856357645426	0.98165991409909	0.09783360814624
C	0.62009308296610	-5.32352830461581	-0.08091454130780
C	-2.66346078208617	2.46044049350761	0.59135896138887
H	-4.14398948028053	3.96520919660672	0.15507551761634
H	-3.86546604851758	3.70432977416380	1.87292389869125
H	-2.11000373289729	-3.94716483253014	-0.28601349433886
C	-2.13092547308226	0.26874929121159	0.27090062237131
C	0.18737960201721	-2.59612640840853	-2.57387948523681
H	-0.58425931836908	1.47658720054139	-2.50904969284565
C	-4.51776608401220	0.78125749993800	1.11568353303388
H	-6.64501318676542	1.27342108633597	2.62380170509225
C	-3.36192227350155	3.74705754766894	0.89672204081892
H	-2.66155636788245	4.59130004210834	0.91565610739956
H	-7.39815346854404	-3.35627288796676	0.56714364515366
H	-7.28700055537592	2.43102502407057	1.40414405938044
H	-7.18117438669177	0.67365493239374	1.02906636686068
O	0.59729416072927	-0.24485659495754	-2.46786467245186
O	-5.41308968580177	1.77156314204939	1.01949435949082
H	-1.82713783199585	-3.30883851474408	-2.56158664139073
O	-4.80910342602068	-0.29042064080408	1.60821259800461
C	-6.70565542808161	1.51447396648153	1.55322179238556

S2.7) Tercer estado triplete optimizado, T₃

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Coordinates from ORCA-job opt

C	5.18837221130229	-0.70651694570752	0.40307814346617
C	4.66333767557163	-1.94716252636188	0.66044154905154
N	2.88047737996939	-0.49199329290012	0.39276034811009
C	-1.13305747958306	-3.42659955703895	-0.34915373519175
H	1.39763848850313	-5.65172897268329	0.76274406729358
C	3.21322257185040	-1.79498924911498	0.62681616460400
H	6.34703195607982	-3.03300265256413	1.42566198070084
H	4.78786289379923	-3.87397875652124	1.60847641403482
C	4.04699790666986	0.20549279264428	0.25018593264727
C	-0.95071641048534	-3.57192896375062	-1.87653690429064
H	-0.37275095397577	-4.15405878632233	1.50257808431540
C	1.03063533829342	3.32600342416717	0.06397566466046
H	0.03539132390167	1.05945375298959	-4.00236308832947
C	4.14022056051422	1.56461745590531	0.00549654875463
Zn	0.98920050250791	0.25437905595252	0.20844924616207
C	-4.26112398995544	-2.46801651487001	0.65312547955705
C	3.05459113560362	2.49845189522303	-0.04784986782510
O	-1.48725478576318	-1.04912594351485	-3.33791199377559
H	0.85907622569954	1.68421085402756	-2.52431570090537
N	1.74626027451778	2.15492342900888	0.06773547913338
C	1.90760216570070	4.44139407584192	-0.08322507633058
H	5.10167143780912	4.57322084120743	0.62903466106858
C	3.19623206301494	3.91487566071191	-0.15497708647207
H	5.10339105143948	4.26580181720321	-1.11331631126557
H	-3.36217120967762	-2.39092266536739	-1.23902057026394
C	4.48995436140146	4.65356038413090	-0.28470605562681
H	4.31914199573813	5.72267701698450	-0.47091279656196
H	-0.81844415424871	4.37949039335721	0.25479259324863
C	1.50519240251454	5.88491987792323	-0.08532902999154
H	1.11952256011075	7.55020510414952	1.27762846181446
H	0.67479129331235	5.95389054892109	1.93086987976719
H	2.38382828435350	6.42609256455411	1.83576704802276
O	-3.76414362186547	-3.01229363033221	1.60798269942101
C	1.41489637438888	6.49057031062150	1.31788751254534
H	2.22873438105353	6.46218795185875	-0.68189240498413
H	0.53520096857489	6.00162435627950	-0.59409259097678
C	6.58209299503336	-0.28413542634290	0.31688296451499
H	6.77368746496066	0.76785280604207	0.55290356833386
H	5.13886018429288	1.98478693662564	-0.10968049514747
C	7.62771170872891	-1.04636616242405	-0.02704901402467
C	-3.51132776320815	-1.69153100850796	-0.40302173000666
H	1.03328455492951	-2.59903630687194	-1.95441942161286
C	5.37709796286568	-3.22517814945760	0.94594263024657
H	5.57876490696019	-3.79476636222799	0.02348744668846
H	0.35556730351013	-3.06884764329592	-3.51261991345043
C	2.30369827623797	-2.84494455208441	0.74401827198572
H	-0.07465110214440	-6.05520332745205	-0.13704321891042
H	8.63675071258702	-0.62798675105043	-0.04720405089622
C	0.92186728726037	-2.76810115414270	0.58145905130527
C	-0.42706051149376	-1.27370745882032	-2.80766578195152
H	7.51833977982598	-2.09280906895582	-0.31792798201892
C	-0.37608450649375	3.38369640801382	0.22253698635835
C	-2.18290071209904	-1.11735173487614	0.02889443834817
C	-6.38066173864562	-3.23477924137086	1.29672401085654
C	-3.20704698259361	1.19953143160506	0.49907790249534
O	-5.55871975848074	-2.54839107276551	0.36031215710782
C	-1.25342494276409	2.31986504203024	0.33505881142662
H	-6.02150566001776	-4.26089232636924	1.45531775007141
H	-6.38217733492962	-2.70271612312288	2.25862456360895
N	0.19502593712692	-1.64006351448839	0.42057954129536
C	-1.09288003186929	-1.96927523908747	0.06176830343176
C	0.07496861108958	1.02222400171541	-2.90546597087664
C	0.03386204924048	-3.98703905541403	0.48814673427469
H	-4.17611277098710	-0.92445229797101	-0.81449867175935
H	2.72074651980602	-3.83891282880079	0.89475118038158
H	-0.70803790924098	-4.61907192916042	-2.10092796689121
H	1.23256096506929	-5.13980904786444	-0.92926873448480
N	-0.93398474609143	0.98832863742021	0.25757507333237
C	0.68569657935519	-5.27506051873176	0.01482437776622

C	-2.69421596492130	2.47140038146713	0.50206554889995
H	-3.25895577655614	4.41283357286727	-0.19525134034030
H	-4.45336013931296	3.64982572556308	0.87643209122179
H	-2.07174861344089	-3.91179727359867	-0.06374967005184
C	-2.09549601215366	0.27681882528821	0.30272468368935
C	0.09805238624877	-2.65936966280502	-2.52233037597507
H	-0.89841394583828	1.31400386080464	-2.49310952994614
C	-4.58407100762947	0.82944297424477	0.88206826664883
H	-7.01301907110046	1.45655707677933	1.73810413885402
C	-3.38096436393434	3.77868849701341	0.69733565084849
H	-2.93956201052629	4.32993186222811	1.54157894191341
H	-7.39032497782750	-3.24690349889764	0.87188793990465
H	-7.48317765544089	2.01977046128810	0.09292390628852
H	-7.13515596450596	0.27890358007495	0.39765151822542
O	0.42833152334250	-0.29607018212454	-2.47399865914738
O	-5.51571232821487	1.57889928837278	0.29257496931869
H	-1.90997418924834	-3.37322757674821	-2.37570198230932
O	-4.85733680463687	-0.04482866077554	1.67354768703363
C	-6.86824359076542	1.31197768054876	0.65872865753644

S2.8) Cuarto estado triplete optimizado, T₄

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Coordinates from ORCA-job opt

C	5.14705272218059	-0.71598590342903	0.52832130280696
C	4.61759945750660	-1.95861121084068	0.76622011416830
N	2.83792178872343	-0.52218897836467	0.41674935544597
C	-1.14643193372438	-3.44758975386109	-0.47914586416457
H	1.39311518331742	-5.69705382732683	0.56133184974798
C	3.17187476351491	-1.81366398445840	0.66817494395132
H	6.27225319159112	-3.03064957432740	1.61221140621459
H	4.71239052729068	-3.87974637432280	1.73123000455857
C	4.01319945243179	0.18988741041188	0.31973926637492
C	-0.93657818322206	-3.50259077907835	-2.00844973746886
H	-0.42572642480561	-4.27204374229858	1.34822826553778
C	0.99926294443462	3.29512376166916	0.01553764716401
H	0.19942773455844	1.12025938282754	-3.94702864730619
C	4.10569826677752	1.53509899886191	0.05964620943825
Zn	0.95710143525805	0.23837763586865	0.19161608616989
C	-4.24510249607028	-2.52897953063979	0.62792269996437
C	3.02460250581126	2.46814263186406	-0.05524452886013
O	-1.41829644557697	-0.82427500174998	-3.16847465357635
H	1.21778039395983	1.69947575066065	-2.57597069791167
N	1.71261907736459	2.13025411712853	0.07824311702657
C	1.86944917634482	4.40078291197338	-0.18903178881112
H	4.97804474183491	4.75058040884572	0.55793480417391
C	3.16385195389546	3.87206936899307	-0.23479248668347
H	5.14205649576745	4.09838820172046	-1.08019618744413
H	-3.38203013060674	-2.37699714450538	-1.28137868879837
C	4.44970234313737	4.61844725406765	-0.40117916075471
H	4.27345185037260	5.62195288523603	-0.81330934332897
H	-0.84173100533200	4.36143576610432	0.21437687690184
C	1.47061230654394	5.84320010977090	-0.26949231006136
H	1.14165851612101	7.59590393712252	0.99503355374685
H	0.70864702894378	6.04835071857148	1.76385015138570
H	2.41658152213044	6.49944148768146	1.58300162635579
O	-3.71703629554174	-3.07075492612233	1.56676895301480
C	1.43145921007768	6.53857482190204	1.09387418491031
H	2.17528359043735	6.37730849928311	-0.92632268256631
H	0.48444005942738	5.93287719027338	-0.75154197247619
C	6.54333207588197	-0.28991979596237	0.50288807704144
H	6.72321638224841	0.76092111304722	0.75303681809526
H	5.10737463418444	1.95570596874133	-0.03093971473969
C	7.60245958325973	-1.04934033258270	0.19824977421866
C	-3.53758163491687	-1.70543533811814	-0.42338903863354
H	1.06959920582145	-2.57765353438060	-1.99407040405927
C	5.32602816749399	-3.23146751091215	1.09055730828813
H	5.57189148573450	-3.80556063381786	0.18189576544778
H	0.39194198097711	-2.88158275984762	-3.58878545481985
C	2.26244808300750	-2.87154390021867	0.74060750826211

H	-0.06047962291853	-6.07979939942459	-0.37636787489329
H	8.61125435184110	-0.63047456438595	0.22151373621643
C	0.88246486654280	-2.81972944834677	0.53594212816913
C	-0.34128663803536	-1.13991863688978	-2.72852500557345
H	7.50562762909347	-2.09454667162832	-0.10148798833335
C	-0.41035831571833	3.36050268606905	0.18614529046120
C	-2.21575400959868	-1.12635111581681	0.00497250363400
C	-6.33176833796416	-3.36343564928433	1.28802741497029
C	-3.23676136437778	1.17719827981447	0.53857599563634
O	-5.54104040728540	-2.64570918889527	0.34778480847357
C	-1.30077156548386	2.30725422040711	0.32125623217011
H	-5.94038286167042	-4.37938699453360	1.43540704811875
H	-6.33864391120186	-2.83784529314365	2.25349830614000
N	0.14280419252583	-1.70079184303261	0.41341326746326
C	-1.11550060992672	-2.00964606730227	0.00844780155500
C	0.33801665812379	1.11325100238284	-2.85797877145893
C	0.00526238178401	-4.04208212657220	0.35537674347236
H	-4.22513032425195	-0.93673230315345	-0.78889697478463
H	2.68826715348112	-3.86415602855860	0.88563680141395
H	-0.69796492019458	-4.53502723524632	-2.29823080607489
H	1.23909282377862	-5.10175272566800	-1.10384413457055
N	-0.97864832047170	0.96704062767441	0.22061950944204
C	0.68276580684753	-5.29434959574374	-0.17495031713027
C	-2.71843481651077	2.45672155953736	0.53156946802701
H	-3.81823129330865	4.14055432748517	-0.21966494865108
H	-4.28342209477853	3.64438060955391	1.40868346381608
H	-2.08310272340737	-3.96056777687178	-0.23819947263553
C	-2.13793065772006	0.25879004597360	0.30159473394793
C	0.13484414792142	-2.56054828309906	-2.56555847084082
H	-0.55733071381180	1.51635583226864	-2.37011040615411
C	-4.59652395267615	0.81686477685957	0.96752000395839
H	-6.91192227534577	1.46971159318272	2.10260916188963
C	-3.42544468233064	3.75617568126007	0.73541712691517
H	-2.75312586812742	4.51828082412790	1.15025896988970
H	-7.34516894223969	-3.40290999486231	0.87388864793250
H	-7.46776033108105	2.25110733613365	0.57869435347920
H	-7.20276720546916	0.47073259487485	0.64947357966234
O	0.59598263996276	-0.22460930817551	-2.41124267721286
O	-5.52105017445269	1.69256758584873	0.56687043706458
H	-1.88335312076387	-3.25894036107780	-2.51237270472837
O	-4.87516659979438	-0.14880925115704	1.64577924288313
C	-6.85459927955265	1.45014348395466	1.00540946829275

S3. Derivado piridinio del trimetil éster de clorina e6 (PyrTMEe6):

S3.1) Estado basal optimizado, S₁

99	Coordinates from ORCA-job opt		
C	-4.28532944350283	0.26342936144358	-0.42057471332380
C	-3.81828012979738	1.53290260236353	-0.11468295251794
N	-2.06240255428548	0.12488512547956	-0.14561319880652
C	1.97237289510502	3.32367957221582	-0.19066947042488
H	0.78697959446887	5.87913205917904	0.25714900033961
C	-2.39823199550061	1.42534481959888	0.04887098982574
H	-4.05447486220499	3.65114212274117	-0.40162292176433
H	-5.56252461006047	2.73152422861135	-0.51784454055287
C	-3.16868334359893	-0.63521347219033	-0.42309580151384
C	2.01203307267322	3.65086574779102	-1.69787270413872
H	0.93547587816775	3.77379167267356	1.60322804940968
C	0.00010639449334	-3.51117419030059	-0.23839903335069
H	-0.08690433289099	-0.85398581703172	-2.31164471419741
C	-3.15454459845266	-2.01329615449090	-0.59042966882966
C	7.01103199726281	0.05343563201640	2.31167811762799
C	4.89127528335322	2.47229101774576	1.19887526646492
C	-2.03280984710595	-2.83695015139716	-0.50957945440154
O	1.89986388791681	0.96663240441716	-2.93665623036920
H	0.15446719050458	-0.54832904982602	-4.06287132653917
N	-0.76227265910245	-2.39955439780255	-0.28257515548507

C	-0.79481502087430	-4.71896865361729	-0.45174697785179
H	-3.86665779770630	-4.74381331654279	-1.74639008212228
C	-2.08096300951641	-4.28965986638943	-0.62345020031176
H	-3.07194086543042	-6.15755476068053	-1.01962857352187
H	4.35707614480427	2.49972561207831	-0.82387579815734
C	-3.31454058924207	-5.09822223505419	-0.86218144917495
H	-4.00675724514607	-5.04096435698485	-0.00683530854213
H	1.86170717738156	-4.51186908487236	-0.00341816290341
C	-0.27854849390299	-6.12524132248273	-0.42567140003346
H	0.54438743010154	-6.09243972581722	1.59777189697161
H	-1.12135190385803	-6.70122325284911	1.50079863680304
H	0.23291550154800	-7.72738765065350	0.96617538313017
O	4.20664681949634	2.77154610379971	2.14500174152867
C	-0.14710172996074	-6.69497619300028	0.98931541769791
H	-0.95178217698852	-6.76714472933807	-1.01370752377436
H	0.69918845087826	-6.17265300103450	-0.93057622935679
C	-5.67473579535864	-0.13553450854516	-0.67050611366356
H	1.02508196047696	-0.72348762987170	-0.01790540533110
H	-4.11678714583489	-2.49219293566779	-0.77202329119708
C	-6.11420345565860	-0.87055956489974	-1.69097432320190
C	4.41921521813599	1.73721042887208	-0.03379714299426
H	-0.11919321924740	3.38829429129455	-2.17638591711181
C	-4.60461479760694	2.79618554885317	0.01454034731372
H	-4.82065966792044	3.03024032283893	1.06996695922229
H	0.94728528304110	3.57785144275873	-3.56090262271129
C	-1.52012464080777	2.48718157295882	0.31811984010898
H	-0.33046638185517	5.08355821836577	-0.87548469502778
H	-1.13108311089997	-0.28237098109093	-0.07080632715358
C	-0.14290743961375	2.47648769334399	0.34626690578957
C	0.89914599504760	1.62939887626384	-2.80529944659255
H	-5.35195777043496	-0.29051374715027	1.86434411356638
C	1.38814359286933	-3.53021705344194	-0.02473063622071
C	3.09305597219345	1.03429646410056	0.11253490278005
C	6.71124516775535	3.63094357228455	2.12940923107864
C	4.16595348348754	-1.29598734047206	0.43518925906410
O	6.17219231303942	2.82402809111692	1.08588255177767
C	2.24796142811121	-2.46718566586579	0.14659038317922
H	7.76697065840648	3.78704407703691	1.88323794046649
H	6.18612222008572	4.59509227360059	2.17831633821256
N	0.66744858312574	1.39504044474013	0.20407822059401
C	1.93561750042729	1.82306155636999	0.06259727619446
C	-0.43397080537310	-0.27320944944760	-3.17717120402268
C	0.67986273564591	3.73851547241684	0.52829626632026
H	5.21812176358892	1.07196975799541	-0.37627661258846
H	-1.9994391549525	3.45499677726253	0.45690601903659
H	2.03763915980899	4.74526575025719	-1.80178847566884
H	-0.78864651317426	5.30655630653090	0.82519343237751
N	1.94912177410683	-1.12445675273992	0.12633173155389
C	0.05008624131388	5.06910475224933	0.15502744478302
C	3.66862121037211	-2.57767592558179	0.34508107494074
H	5.46248360102071	-3.71366230195309	0.67124078667810
H	3.96771825692641	-4.48823481242885	1.27339078525561
H	2.83711539005726	3.80220521013929	0.27859192724458
C	3.06979207475971	-0.36371182594077	0.25570875121533
C	0.87000570710060	3.11689279779620	-2.56167972870987
H	-1.49742491149544	-0.47368760744741	-3.34833422093822
C	5.57527214327134	-1.03314561023492	0.80787838040904
H	6.90431811876505	0.72423054333259	3.17003420708867
C	4.39810182500238	-3.87238573865237	0.47004463302549
H	4.31365331200703	-4.45032206923899	-0.46288892480436
H	6.61773062970756	3.12622683122480	3.10034403093490
H	7.47161401285964	-0.89373620384222	2.62207598638944
H	7.62944525506975	0.52216290386162	1.53520981739836
O	-0.32935091061157	1.12334202126366	-2.91561672923859
O	5.68831865686998	-0.17660442698211	1.82489381006414
H	2.95834395971169	3.28178093094354	-2.12011268392304
O	6.52636571592114	-1.58882554613776	0.31262013420913
H	-5.42026753855950	-1.16910414820721	-2.47689707244848
H	-7.15389480014702	-1.19413181323844	-1.76750354196303

C	-7.80643467000559	0.85780709978315	-0.03758113108213
C	-8.72442589728247	1.26816132508253	0.90725515039703
C	-8.42214806861719	1.12167444232752	2.25824744123796
C	-7.20135656707919	0.56059505967211	2.62682722753374
C	-6.31949159478020	0.16100450272797	1.64534084044113
N	-6.63160640639382	0.30969144278237	0.33912271770308
H	-7.96638995613532	0.97246115801026	-1.10894064753064
H	-9.66306926325156	1.71254244143658	0.57609960929828
H	-9.13196440497552	1.44719587937789	3.02097976004731
H	-6.92687588050145	0.42617867800634	3.67315375135895

S3.2) Primer estado single optimizado, S₂

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Coordinates from ORCA-job opt

C	-4.28938780232120	0.24521946782870	-0.39817483795932
C	-3.82211368080026	1.51492901623341	-0.06681934739141
N	-2.06170334743437	0.10228689759115	-0.13543032621614
C	1.96468101519159	3.30090028914122	-0.20284308635924
H	0.78661690615401	5.84277117174636	0.29666358724090
C	-2.40172663478328	1.41050624045155	0.08833115401669
H	-4.01507682278147	3.65573040801515	-0.16461442576612
H	-5.48772390322880	2.77085050551754	-0.59400155006626
C	-3.16314959180157	-0.64930181271783	-0.42246040301140
C	1.95104520989374	3.64146097184650	-1.70889065618329
H	0.97236069229182	3.72658013559828	1.62244499057579
C	0.02722775999126	-3.51438709402512	-0.25148637912097
H	-0.08765504815020	-0.88818425518462	-2.32547623006517
C	-3.14475603211413	-2.03518067113804	-0.62014160318025
C	7.00082226842156	0.09631659029949	2.34524415665759
C	4.91404265240102	2.49007877092395	1.16348107264074
C	-2.00947457869050	-2.83706405992727	-0.53162153380053
O	1.85099291344019	0.96419768720692	-2.93086223621062
H	0.11209405454339	-0.56328557798309	-4.07870431385419
N	-0.74532039034363	-2.39790421827148	-0.29411539177662
C	-0.77898227567335	-4.73415630243195	-0.47672453702851
H	-3.78081383955994	-4.77241043486402	-1.85159778984518
C	-2.05227366149954	-4.30743354661842	-0.65825187669452
H	-3.07123966349081	-6.16873830906069	-1.00629334620794
H	4.36502837571835	2.49819228775781	-0.85570263026559
C	-3.28986319712835	-5.09640861469830	-0.92035087698258
H	-4.02507591990730	-4.96609006357047	-0.11026226906487
H	1.87161512736668	-4.52960312430247	-0.02586369133691
C	-0.25416998677179	-6.13518054960715	-0.44674925991909
H	0.60246107211161	-6.07064070169549	1.56371097170074
H	-1.05792242216692	-6.69875770961700	1.49994533300864
H	0.29945560797253	-7.71422599501609	0.95212174502772
O	4.22880372194081	2.81688207186425	2.10049398129165
C	-0.09220990895868	-6.68640385051577	0.97296241675464
H	-0.93468068717776	-6.78699763426024	-1.01443479565166
H	0.71471915670762	-6.17826522494248	-0.96876437935993
C	-5.67378880142631	-0.15201308499716	-0.64431164190545
H	1.05281474697751	-0.73153087349085	-0.04090711503737
H	-4.09904933842901	-2.52162564740158	-0.81207470362491
C	-6.12610063735332	-0.93177711465667	-1.62805293638280
C	4.43423484657787	1.74231939296059	-0.05871213451191
H	-0.19130965528161	3.34142484869087	-2.11127315188565
C	-4.61728842641403	2.76980619432007	0.07659112347135
H	-4.98983503988568	2.90136357386198	1.10694146423500
H	0.81707760783745	3.56821218223057	-3.53102150134891
C	-1.52002675518816	2.46092119614799	0.36684587288505
H	-0.36806728910572	5.05837888102440	-0.80570539637706
H	-1.12978951515880	-0.30589324744522	-0.06793531409433
C	-0.13083381079029	2.44107032079422	0.37500419086614
C	0.84026497137311	1.61059168638973	-2.79305207630991
H	-5.43031192573435	-0.30221876253242	1.89585364438462
C	1.40105111173839	-3.54746167332630	-0.04282660831490
C	3.11395558280482	1.03586123162954	0.10591141884609
C	6.74025719699231	3.64978579906864	2.07880148442370
C	4.18897487543900	-1.29735391766347	0.45474874204260

O	6.19962402246717	2.82379894981751	1.05106601055565
C	2.27610732517642	-2.47155840974825	0.13302841727339
H	7.80056385861857	3.78424970008014	1.83965676744874
H	6.22864157903790	4.62231023308311	2.09711812961850
N	0.67259278767040	1.36272590574886	0.19951292493469
C	1.94918393520812	1.80635687031281	0.04762162698589
C	-0.46350976380621	-0.30768779466979	-3.17876686006452
C	0.68632919012544	3.70261132829106	0.55475588806983
H	5.23081315655115	1.07246063561128	-0.39910070066866
H	-1.98852195426013	3.42870297958302	0.53482773946908
H	1.95790035860103	4.73667359881157	-1.80337966297084
H	-0.77189860704886	5.26937527341682	0.91047967789807
N	1.97550198360338	-1.13468043440055	0.11092774724627
C	0.04439157146101	5.03562513521885	0.21217577569359
C	3.68664567795412	-2.58747549786010	0.34674515011839
H	5.46933224268501	-3.73189037450868	0.69321933315856
H	3.96404867529239	-4.50884713423705	1.26536057574209
H	2.84003564438358	3.78390219646742	0.24111720648017
C	3.09914600608289	-0.36999708757946	0.26407357414151
C	0.78932672322264	3.09481449673372	-2.53501117765500
H	-1.52617407589331	-0.52706017456534	-3.33020180418128
C	5.58662735537093	-1.03833925292932	0.85584359336877
H	6.88369930519672	0.80456760744005	3.17162655590542
C	4.40796833550567	-3.88596104939154	0.47373321536634
H	4.33799342933214	-4.46020243736105	-0.46379382336587
H	6.62955427890555	3.17260983426388	3.06168396762976
H	7.43292431184515	-0.84537540356478	2.70867109593717
H	7.65246652468358	0.51975376431379	1.56981859335274
O	-0.38031763254217	1.08853989336621	-2.90697381550835
O	5.68910224090445	-0.12870993889573	1.82972531463834
H	2.88934779027765	3.28679339140988	-2.16002489470574
O	6.54473303856769	-1.63756120040423	0.42507187282194
H	-5.44145642089177	-1.27689086174420	-2.40287236554560
H	-7.16981555742960	-1.24676040498305	-1.68136931929231
C	-7.77301047368677	0.94988879837039	-0.07853866403623
C	-8.69839090992071	1.40712703066717	0.83772330318317
C	-8.44343634490849	1.25077004093265	2.19724701321213
C	-7.26148464830494	0.63476907818329	2.60394108887717
C	-6.37027958689532	0.19194627775342	1.64975368377550
N	-6.63755611697566	0.34965640430383	0.33522753490897
H	-7.89614478418026	1.06326476676215	-1.15515355774609
H	-9.60538435257995	1.89322934929837	0.47823224091114
H	-9.16005612885921	1.61067711098017	2.93782752178086
H	-7.02574587986281	0.49089305844252	3.65840050827852

S3.3) Segundo estado single optimizado, S₃

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Coordinates from ORCA-job opt

C	-4.28201330406652	0.24457396712374	-0.36383587720226
C	-3.80636555695928	1.53111070810945	-0.04056711757976
N	-2.05890799162716	0.12050924931792	-0.14137963071482
C	1.98756496536468	3.30992428191452	-0.26354224023801
H	0.81562013213994	5.87790489116179	0.14037707303075
C	-2.40309176568208	1.42496121436381	0.08441426998966
H	-4.00407467438468	3.67831994286748	0.00070944930811
H	-5.40442803033331	2.82667675287007	-0.66807325622853
C	-3.16336755187761	-0.63272817518898	-0.41258718988150
C	1.99409465100345	3.59066408020813	-1.77972978533580
H	0.99614083842224	3.81265990671077	1.54301664172345
C	0.03744336178693	-3.52480477543017	-0.33778162479591
H	-0.16203420779555	-0.93498909741483	-2.35290595503638
C	-3.13170891612999	-2.02373312465455	-0.62960689157120
C	6.80216379233610	0.19879421206530	2.62339160340181
C	4.91411479968751	2.51829344862064	1.11461111815067
C	-2.00161631424044	-2.83240214642098	-0.58334387746474
O	1.84775549512961	0.86244407719184	-2.90962050656058
H	0.08997877000917	-0.61735322368151	-4.10071923586918
N	-0.73404941217916	-2.40097353825728	-0.34626941712744
C	-0.76799133117801	-4.72626654316963	-0.59586958909881

H	-3.80108550422942	-4.71675265948583	-1.92687769752837
C	-2.04717494469905	-4.29012128134678	-0.75156344795628
H	-3.05798071046057	-6.14307358761904	-1.16709840521183
H	4.37472484166858	2.41749750168189	-0.90392699940805
C	-3.28486802761711	-5.07845494804143	-1.02373999166542
H	-4.00243505182721	-4.99848071476824	-0.19152731955789
H	1.87294120433375	-4.54459281660343	-0.09690018301414
C	-0.25149208694648	-6.13183714650096	-0.61683174869827
H	0.57664130458075	-6.15915337249858	1.40517271199157
H	-1.08686457568095	-6.77124955976354	1.29288106154314
H	0.27040267754042	-7.77389524231211	0.72175308860597
O	4.22788244302917	2.91563813123406	2.02201047375455
C	-0.11395949677086	-6.74462549026446	0.77967239648114
H	-0.92701646090459	-6.75511300840656	-1.22170007288764
H	0.72435844360029	-6.16054573268609	-1.12663756257733
C	-5.67164737111948	-0.14484776047046	-0.58387491646179
H	1.07112425432343	-0.76645425344620	-0.14693464998395
H	-4.09027434939641	-2.50672167305256	-0.81713108225512
C	-6.15808566846324	-0.89908423367386	-1.57102911489376
C	4.43438710478493	1.70378456815878	-0.06769236059662
H	-0.14665539461075	3.31703652416317	-2.20748606288732
C	-4.62059259082488	2.77616868801363	0.10203680527848
H	-5.11907069294803	2.83169109776498	1.08446516832540
H	0.88938016666448	3.46801640234578	-3.61698805656546
C	-1.49305073712715	2.48649533882683	0.33422762059362
H	-0.32651490169071	5.05048946766419	-0.94392044947918
H	-1.12395974062794	-0.28312373318016	-0.09010388139649
C	-0.11841858123236	2.48188533498595	0.34357571242729
C	0.85369934937381	1.54160774980661	-2.81407642823842
H	-5.35924809918404	-0.37414290674047	1.93989092778884
C	1.40372485829916	-3.56037876731528	-0.10809352159896
C	3.10647115122925	1.02513589551836	0.11609662397408
C	6.75463096233292	3.71365402834928	1.95207803488869
C	4.15948021511353	-1.30250489352605	0.58006459789821
O	6.20543531251303	2.81771408099445	0.98812536746324
C	2.29007062196550	-2.48959975561676	0.12345669045596
H	7.81816072555814	3.81057472978246	1.70961336493512
H	6.25922547027004	4.69254887408745	1.88816777721104
N	0.69099111521911	1.39214848318309	0.21839454256547
C	1.95744712527749	1.81900098812260	0.04269606604286
C	-0.49853655496070	-0.34297118872620	-3.21472113313771
C	0.71221495245555	3.74606553084657	0.47671875225880
H	5.22538799063847	1.00405632247260	-0.35603823930708
H	-1.96515866299073	3.45850611818542	0.47380964890305
H	2.01837742701643	4.68141784812589	-1.91758360840763
H	-0.74838558350121	5.32499938443349	0.75854789465861
N	1.98602660207692	-1.15391189871186	0.07464259952268
C	0.07602219199523	5.06623674107158	0.07829767648244
C	3.66471844406256	-2.60759211576306	0.43557830175316
H	5.41629394403919	-3.74217835079280	0.93689090287879
H	3.87410795128300	-4.53319701994050	1.36992507744472
H	2.86003782299342	3.80548899813247	0.17140951467758
C	3.09040800322611	-0.39233444815244	0.30835078443312
C	0.83499810979681	3.03414205605200	-2.60397008384431
H	-1.56367524543937	-0.52926822662804	-3.39134026079066
C	5.51422699362359	-1.03304870391924	1.09598700269664
H	6.61940394867442	0.97063857268947	3.37793119090825
C	4.38061124144591	-3.90424686815691	0.62238616742385
H	4.40234445176131	-4.47561166962460	-0.31915660593889
H	6.63021162903640	3.31774338594750	2.96857579307163
H	7.17682257593090	-0.71740590800195	3.09847194203548
H	7.53588644596688	0.55073337160319	1.88625527948904
O	-0.37894015542175	1.05129476235596	-2.94395260085201
O	5.54274604302824	-0.04730519205559	1.99994186899379
H	2.93193783856177	3.20845761385742	-2.20978532759258
O	6.49835962359558	-1.67735454030536	0.81305005197259
H	-5.49963643978253	-1.22609364686678	-2.37586981070143
H	-7.20358329946024	-1.21149779466041	-1.59660912207250
C	-7.74120535193365	0.96454120713310	0.07397892621167

C	-8.63135723991023	1.41115195649278	1.02992943163349
C	-8.33792651917457	1.21387379726063	2.37619636916697
C	-7.15458646890526	0.56840639995304	2.73022509873569
C	-6.29950825507234	0.13897903502262	1.73769432944343
N	-6.60393372972481	0.33706525095769	0.43692043081194
H	-7.89410899562117	1.10779232333445	-0.99515702207806
H	-9.54077131233807	1.92075017952598	0.71151743134874
H	-9.02568592418916	1.56486765597506	3.14778918012658
H	-6.88986160352516	0.39212860520466	3.77284312737822

S3.4) Tercer estado single optimizado, S₄

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Coordinates from ORCA-job opt

C	-4.26882322446537	0.36437490313408	-0.46230472732577
C	-3.79849226847990	1.62786725339152	-0.17584508431971
N	-2.03882092783424	0.20031657000749	-0.18695500442186
C	2.02443126835595	3.33466023903271	-0.27083983901257
H	0.87187303931826	5.91153118925595	0.11134998908868
C	-2.36426174336683	1.51446573352788	-0.00745473357954
H	-4.07973722740831	3.73136715667798	-0.51857166336130
H	-5.58065713876514	2.77192392962381	-0.48972664182199
C	-3.15421909936087	-0.53461052234325	-0.45243353877463
C	2.06384939334393	3.62851372790479	-1.78709247266576
H	0.98464521662377	3.83722220424719	1.50995924211637
C	-0.05935747943695	-3.45028200950878	-0.23204061049271
H	-0.07981517890772	-0.86142130124820	-2.34842276953050
C	-3.17446592026453	-1.92956454914005	-0.62283469746816
C	6.95083902640847	0.00546669869681	2.42622192088211
C	4.88681640424258	2.45616882626164	1.21259910086519
C	-2.08016684765056	-2.75932307207094	-0.53129408498776
O	1.90385831746088	0.91156816197484	-2.92224040266800
H	0.11220291425838	-0.56880846239538	-4.10665594014691
N	-0.78837390759083	-2.33813213819927	-0.28539847725141
C	-0.87038086454625	-4.66228799956571	-0.45566660286599
H	-3.89476741430875	-4.64736521658314	-1.81851945587282
C	-2.14150508094719	-4.22181851031935	-0.64773511195953
H	-3.16841631070466	-6.06954027450388	-1.03266998129471
H	4.41777387982535	2.46606470264401	-0.83145009632747
C	-3.38534234952255	-5.00082153503231	-0.90886450645784
H	-4.10121834963789	-4.89648118611612	-0.07832149914700
H	1.79756402043691	-4.48483077983639	0.03458670931813
C	-0.35876110192931	-6.06780342676322	-0.41552646942159
H	0.49247998188774	-6.00160247029114	1.59890064072390
H	-1.17482873196107	-6.61022643922750	1.53154388123027
H	0.17295618357292	-7.64399332356221	0.99379428900679
O	4.15802405124241	2.79802922862986	2.11026480959831
C	-0.20731046759487	-6.61194914138290	1.00802743672714
H	-1.04440346064824	-6.71533462806054	-0.98152927786283
H	0.61065172540460	-6.12413940853527	-0.93562601781465
C	-5.66890029988871	-0.03366877658538	-0.69681439346727
H	1.00458724687921	-0.68964374942577	-0.04027292503822
H	-4.14983399417862	-2.37522670199260	-0.81574739283100
C	-6.05799693935570	-0.58931827490581	-1.85950260134925
C	4.44961748088171	1.71360072980874	-0.02980629692862
H	-0.07451948434734	3.39148108544992	-2.25581917436696
C	-4.58612512020714	2.88188816138780	-0.03870562634978
H	-4.72606087087916	3.14074728902905	1.02424568563113
H	0.99129746832187	3.52665903348857	-3.64226707548717
C	-1.49198198934174	2.56054870103910	0.25113928296302
H	-0.26463449599742	5.11028217275071	-0.99760019968082
H	-1.11425008631161	-0.21835362969403	-0.09968483041956
C	-0.09698949943186	2.53057843757772	0.28176361050705
C	0.91390456416942	1.59798066701696	-2.83667236007685
H	-5.05559159012319	0.09089684966036	1.83457925286978
C	1.34121925241808	-3.49645101611963	-0.00166152018723
C	3.10909359080697	1.03627709431711	0.09449820533016
C	6.69403819293468	3.56207929291365	2.22418635410176
C	4.13887748399295	-1.30286760925883	0.47375178988170
O	6.18174342653437	2.75472852603274	1.16542970426544

C	2.20089327138709	-2.44464920208568	0.16524022700181
H	7.76973754555972	3.65836692626833	2.04347298302103
H	6.21612710665609	4.55150201423026	2.21434883745563
N	0.68437272270280	1.43851441044142	0.15518399062708
C	1.96552290344940	1.84702390352462	0.01151927389698
C	-0.44806903793056	-0.28301222024477	-3.20617681458687
C	0.73312006347563	3.78436764300378	0.43452760611820
H	5.24569268709881	1.03146780684711	-0.34356967238219
H	-1.95765942842361	3.53657912205177	0.37624455055136
H	2.10495446932956	4.71975886578317	-1.91107220830014
H	-0.71056262233712	5.38029431106195	0.70046724797980
N	1.92042738155126	-1.09950714508616	0.12868449918251
C	0.11968353948227	5.11370995664189	0.03126009287802
C	3.63204542484386	-2.57136045466532	0.39002119932232
H	5.40154153037957	-3.73296448362751	0.73579624439790
H	3.88913164570485	-4.46492911758485	1.35294103386728
H	2.89645958151113	3.80918498354593	0.18732565265785
C	3.05184688447365	-0.35456052589282	0.26168894906997
C	0.91071057583830	3.09164041648295	-2.63186837951774
H	-1.51789568922091	-0.47260174979764	-3.34624862053653
C	5.54681929897683	-1.04726886657615	0.86984989544697
H	6.82454858258520	0.66446325109638	3.29079668369701
C	4.33417927230114	-3.87432202337709	0.53835847225924
H	4.23303893569144	-4.46615159808246	-0.38433336273988
H	6.51109642572948	3.08741593654783	3.19729450344639
H	7.39226278476644	-0.95109644020048	2.73500240366314
H	7.59286695938394	0.47983216820344	1.67326950514134
O	-0.32132658895873	1.11491861332388	-2.95798334992180
O	5.63882310664248	-0.20704932055808	1.89840497375705
H	3.00419732297948	3.23579433521803	-2.20058668090354
O	6.49915507693594	-1.59928792748302	0.37692919587623
H	-5.33361103240375	-0.69938830135277	-2.66549056291998
H	-7.07645606256745	-0.93580436598998	-2.03522586087067
C	-7.91152863853279	0.42958543521930	0.12203387455021
C	-8.79171240256281	0.64475533077298	1.14668764313787
C	-8.35531087965521	0.67521130041817	2.48354766599745
C	-6.98615171093757	0.48298400161104	2.71635972547888
C	-6.11588441547234	0.26690035863131	1.67953334438811
N	-6.55927021412457	0.23412767031745	0.36495822106346
H	-8.21167324864982	0.44328688562367	-0.92186284880200
H	-9.84057905122444	0.80778169903974	0.89524165366325
H	-9.05140642297303	0.84634765058482	3.30264911867543
H	-6.58119731738835	0.49195633329821	3.72912529114044

S3.5) Primer estado triplete optimizado, T₁

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Coordinates from ORCA-job opt			
C	-4.29508833257009	0.27715087280707	-0.45008987439860
C	-3.82813633853950	1.54010962252953	-0.13915532353649
N	-2.06112178624514	0.12499624862742	-0.16339599214477
C	1.96992737361119	3.32295535245413	-0.21913255398288
H	0.78261444233311	5.87553916297298	0.21860030130637
C	-2.40012183097653	1.43277729959062	0.03252008017648
H	-4.05540432668959	3.65818622775638	-0.41954251888829
H	-5.56689305846264	2.74004615693506	-0.54271574769086
C	-3.17130472389803	-0.63064870522576	-0.44304953692732
C	1.99434879419925	3.64816363519853	-1.72940246436775
H	0.93873651418880	3.77888014574510	1.57749184899869
C	-0.00242920792063	-3.51464945634973	-0.24743267073342
H	-0.06068133927722	-0.87980805616478	-2.32485774411561
C	-3.16743925387240	-2.00640219436070	-0.60741162155011
C	7.00113263153463	0.06024136287378	2.34657252601360
C	4.87756117091096	2.47680296346625	1.21134940726283
C	-2.03907032374059	-2.84102755986032	-0.51872204253304
O	1.90184278789943	0.95709166994872	-2.93707343503209
H	0.16408084783268	-0.57352044714658	-4.07825463082415
N	-0.76443668787325	-2.40011554166043	-0.29352645935190
C	-0.79671968575334	-4.71972105558461	-0.45572919084490
H	-3.87279618092232	-4.74497789342666	-1.75556975600057

C	-2.08925433226964	-4.28668404569697	-0.62802459222359
H	-3.08658144137238	-6.15358668405384	-1.01057023212440
H	4.36612619184566	2.51158612044397	-0.81954738342536
C	-3.32499318016118	-5.09138935883900	-0.86465327507396
H	-4.02395511420785	-5.02344629639418	-0.01461244382220
H	1.87048550725700	-4.51238691922108	-0.00810964874177
C	-0.27944693737115	-6.12399513612526	-0.42569422097267
H	0.57333841162028	-6.07910534980278	1.58670053040721
H	-1.09251432212196	-6.69115225964860	1.51672377484904
H	0.25662304300502	-7.71794104464189	0.96809730684016
O	4.17128456968506	2.78565778398231	2.13839379797209
C	-0.12569070581641	-6.68610131925332	0.99136664300296
H	-0.95997064094475	-6.77226298989751	-0.99875823476666
H	0.69250421302986	-6.17520621746529	-0.94301353171832
C	-5.68600278213003	-0.12384360253393	-0.67975326356492
H	1.02982051680227	-0.72460382502481	-0.03429229986028
H	-4.13167466425233	-2.48099092320245	-0.78926058588156
C	-6.13874471121569	-0.84290349968034	-1.70705468909041
C	4.42422810436317	1.74553686340894	-0.03197480862168
H	-0.13948635722757	3.36075832362730	-2.18339935888353
C	-4.60989624080328	2.80303459149967	-0.00895117254209
H	-4.82591865554276	3.03205319914143	1.04791027311905
H	0.90837121491693	3.55758807028466	-3.57872053289964
C	-1.53039209618686	2.48802802569892	0.30471864845237
H	-0.34603810636836	5.07575860741085	-0.89984649763875
H	-1.13341824775104	-0.28778196833361	-0.07516840804805
C	-0.13826140799923	2.47522339589963	0.33154278780814
C	0.89371088207805	1.61078291500447	-2.81499107683390
H	-5.34796818322101	-0.37721836688883	1.85153987391309
C	1.39687809909826	-3.53119641280809	-0.03459936407323
C	3.10105912512742	1.03912336150523	0.10229373477632
C	6.68474207145572	3.61579799989203	2.18636727595327
C	4.17697434968311	-1.28906359150172	0.44005863023140
O	6.16372818706587	2.81197803142392	1.13035405134172
C	2.25630515370598	-2.46319498343496	0.13202564385476
H	7.74949724278868	3.75391791073159	1.97061773487529
H	6.17299835710412	4.58788714276625	2.21495152206557
N	0.66581966756518	1.39729064192350	0.18673779669806
C	1.93903568773871	1.82877444101197	0.04029146429545
C	-0.42065639218916	-0.30414036979359	-3.18837339412886
C	0.67685203282495	3.73864458434533	0.50306854449277
H	5.22707530115551	1.08150686893662	-0.36810575933233
H	-2.00578945255995	3.45706641070214	0.44715584209902
H	2.00904600766519	4.74249187290133	-1.83442388645587
H	-0.78919314162009	5.30905564448563	0.80385115098856
N	1.95439363685951	-1.12321738090847	0.11342159057791
C	0.04301567702060	5.06676334597311	0.12745006023064
C	3.68318183734705	-2.57217512827041	0.34060096786439
H	5.46996686058500	-3.71718061306526	0.66039261582693
H	3.97224041404861	-4.48020193431824	1.27403864864034
H	2.83667020170076	3.80708775283438	0.24089926498439
C	3.08226344832156	-0.35835377224944	0.25459731954819
C	0.84945028209880	3.09877571384894	-2.57715100455493
H	-1.48325683433392	-0.51598013036352	-3.35071737907543
C	5.58160643190928	-1.02587329285040	0.82696244714698
H	6.88541110882621	0.72964323239354	3.20481926383175
C	4.40326698527108	-3.86876259099152	0.46619549688708
H	4.30679787790490	-4.45227520799059	-0.46324588508042
H	6.55396425341689	3.11687970766020	3.15586270940916
H	7.45244044210609	-0.88975518047890	2.66166256637664
H	7.63294031975171	0.52768595787926	1.58029525876019
O	-0.32899221627213	1.09423265969973	-2.92956970104704
O	5.68447873782159	-0.16330562710201	1.84030037885195
H	2.94101284781483	3.28465108494316	-2.15546684720267
O	6.53728707679972	-1.58738476507013	0.34688900321301
H	-5.45672236653174	-1.12929594016942	-2.50797856851104
H	-7.18002625537502	-1.16388358351995	-1.77319751658377
C	-7.78526218211544	0.90535653607136	0.00169711572732
C	-8.67824524558322	1.31550257866085	0.96874112917059

C	-8.37319361935652	1.11831295747599	2.31426021175554
C	-7.16421294255276	0.50429948184023	2.65180845287889
C	-6.30310382630859	0.10891964622484	1.65447175132009
N	-6.61904621031062	0.30640457543812	0.34923856909532
H	-7.95129053904597	1.05597060176572	-1.06394431356787
H	-9.60468714278718	1.79967290691925	0.65928093020885
H	-9.06523710626693	1.44257778349250	3.09286846528920
H	-6.88607526278216	0.32673117031550	3.69079002988034

S3.6) Segundo estado triplete optimizado, T₂

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Coordinates from ORCA-job opt

C	-4.30306572837615	0.21311089062898	-0.39990124689662
C	-3.83247498377558	1.50535077102329	-0.11475059756364
N	-2.08238080618564	0.09958966978012	-0.12624348561924
C	1.93955508733108	3.32390117488430	-0.15580023900022
H	0.76812607275875	5.86913763577147	0.37073713919130
C	-2.43289698287273	1.40207050774750	0.04798153584305
H	-4.02053267350765	3.65101103052240	-0.19629487662884
H	-5.43662198238784	2.77319262654050	-0.78973813676710
C	-3.18319488680602	-0.67357461633279	-0.39166228371999
C	1.96652275562051	3.68921766220341	-1.65482365319346
H	0.92881407911468	3.73025851339066	1.65964798564892
C	0.04502287351721	-3.55342075950677	-0.22304606580078
H	0.03147545562828	-0.85187256458472	-2.30542716046409
C	-3.15141773266915	-2.05810010645989	-0.54478914498733
C	7.09327953220206	0.04317756335953	2.17128566973520
C	4.85391095384726	2.45433110347186	1.21433458792437
C	-1.99694622828487	-2.86280651080488	-0.45716807132138
O	1.92753051332499	1.02851452211906	-2.91171214059834
H	0.20511658509650	-0.53219422192454	-4.06124228686016
N	-0.75390778849903	-2.41891604856669	-0.25871514956286
C	-0.77177229071543	-4.76787193048147	-0.41403409709137
H	-3.81369383189234	-4.80601205484117	-1.69937864179705
C	-2.04708549726944	-4.33735203477010	-0.56310734556622
H	-3.08108188013356	-6.19862356508800	-0.86773784313220
H	4.33062085261946	2.55199258334334	-0.81488277188184
C	-3.29424585168254	-5.12508016254021	-0.78187188038928
H	-4.00373071314107	-4.98779632752986	0.04988112540647
H	1.88323481031071	-4.54350109101258	-0.04956545984647
C	-0.25444702703872	-6.17231667965497	-0.38840598493127
H	0.62417207744627	-6.11588292440334	1.61240878915793
H	-1.04225602624944	-6.72998446984625	1.56662829798601
H	0.30008910366512	-7.75662508997743	1.00368306458564
O	4.14897742412456	2.69205199244118	2.16350343309369
C	-0.08222039555539	-6.72532218370210	1.02914600733325
H	-0.94477154899101	-6.81997417894906	-0.94921952466007
H	0.70868750761980	-6.22196355927348	-0.92025143592174
C	-5.68735744700657	-0.18551039674982	-0.63909962610231
H	1.04237585989811	-0.75220607168593	-0.02273322870427
H	-4.10308990591387	-2.55856630134671	-0.71276044123412
C	-6.14219475043098	-0.99732031108079	-1.59484380412882
C	4.40721406691026	1.76205510757422	-0.05327499072642
H	-0.15928993362950	3.38369576289757	-2.12845118706336
C	-4.64095993475070	2.76115969037766	-0.03090436346348
H	-5.12137058972279	2.87856979775559	0.95484755565134
H	0.89600737202472	3.61871930522971	-3.51558721274534
C	-1.52719350381182	2.48211281469375	0.31791920240534
H	-0.35934685959034	5.10228727959718	-0.77333452677557
H	-1.14666584341466	-0.29593707241480	-0.04892016951964
C	-0.17808922343586	2.47732379998504	0.37928059505325
C	0.90578042727535	1.65956723661077	-2.78060189755800
H	-5.46045681537185	-0.25424083559348	1.90405072528275
C	1.39680326620773	-3.56819836804443	-0.05629766288446
C	3.10000714109454	1.03045799116760	0.07526723513240
C	6.63355745917138	3.60446033626706	2.22437206395760
C	4.19914890154813	-1.28477134859637	0.35479835617583
O	6.12540777913076	2.83897946547719	1.13400054960344
C	2.29277845415553	-2.46476741255847	0.09544131586111

H	7.69127100618679	3.78568598372886	2.00591817579473
H	6.09301781885776	4.55770242892474	2.30690009043000
N	0.67595879810252	1.37045377085008	0.24019307947230
C	1.90242718270088	1.81895604067425	0.06453641307351
C	-0.36546732459921	-0.28266436092948	-3.15641460130310
C	0.65474764673687	3.72298604732673	0.58891350384618
H	5.21684763244062	1.12041175623501	-0.41468057575549
H	-2.01050760409258	3.44863616741124	0.45147893999770
H	1.96359496105810	4.78595257338855	-1.73005749680817
H	-0.80643307097463	5.28622054737460	0.93482806782862
N	1.97653916229821	-1.14385945053975	0.08388850460909
C	0.02804630107871	5.06398165867551	0.25420763579272
C	3.69524538197556	-2.58100787463481	0.26038699187572
H	5.50295876534835	-3.71062862445163	0.52454648562325
H	4.03918247495025	-4.49955858596795	1.17294866970773
H	2.81033370730355	3.78969727396196	0.31543935721902
C	3.10355150533483	-0.36438670485892	0.20692889470302
C	0.83426558615702	3.14294804477759	-2.52233710304016
H	-1.42541196435889	-0.52264704135537	-3.29456996359921
C	5.61431457494898	-1.02847527105999	0.69821352090044
H	7.01238727729830	0.69306878156193	3.04830981486632
C	4.43369669941021	-3.87603995636336	0.35670816152613
H	4.32775963826969	-4.45437811485815	-0.57404075490197
H	6.52812558563319	3.05351209348413	3.16849832489520
H	7.56356643478563	-0.91023491575130	2.44550324293701
H	7.68945595401402	0.53117311322666	1.38910485717420
O	-0.30530902773355	1.11644263337174	-2.89247481517328
O	5.75757665019154	-0.17721807596793	1.71787396258839
H	2.92018324918941	3.35525312285193	-2.08929709785602
O	6.55298950701998	-1.58594547557903	0.18001768030888
H	-5.45757785868916	-1.37506025178119	-2.35395758233371
H	-7.18823835608826	-1.30515990181431	-1.64018432798427
C	-7.77783992482766	0.95812814754456	-0.12346755257071
C	-8.70407990377124	1.45377107865831	0.77193571114012
C	-8.45969075607936	1.33710632275719	2.13728161388409
C	-7.28687987625626	0.72204421878886	2.57106644042729
C	-6.39448704914749	0.24026756770838	1.63708242136791
N	-6.65243272425965	0.35845819077094	0.31679970139190
H	-7.89300620535874	1.03877439929501	-1.20393162755171
H	-9.60334819827174	1.93825796331693	0.39152138142443
H	-9.17721675030662	1.72757024279563	2.86128781567964
H	-7.05927865500704	0.60945679991207	3.63107143847071

S3.7) Tercer estado triplete optimizado, T₃

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Coordinates from ORCA-job opt

C	-4.26846950684441	0.24778128814293	-0.38606742072884
C	-3.79880707674990	1.51118067320045	-0.02631667642739
N	-2.05164501080902	0.07923511978450	-0.05943432894165
C	1.95637072860757	3.27562102904827	-0.15707230683342
H	0.80071335664605	5.80328587571394	0.44149479395793
C	-2.38285303655397	1.39072927370087	0.17144407277115
H	-3.96831381197398	3.65023138214378	-0.15368313372080
H	-5.45684536616970	2.77646678395292	-0.55271308432487
C	-3.15049828665875	-0.65048540029122	-0.38587663119725
C	1.88079309103947	3.63639447015279	-1.65659972904192
H	1.02680069971164	3.65642173095341	1.71255498192669
C	0.05488447952413	-3.50977332318576	-0.19038602600263
H	-0.26862907532015	-0.86936543051643	-2.28537396045909
C	-3.12228512210862	-2.04477088302526	-0.60640639557067
C	7.08337210210620	0.09862526019528	2.24100683082050
C	4.95693103154375	2.48575882550465	1.09603294274641
C	-1.98291977383079	-2.82101040677083	-0.49454558155617
O	1.71672730943553	0.97092256611339	-2.88037259785030
H	-0.03426924993350	-0.51810233197839	-4.03058833163799
N	-0.72259517301142	-2.38570696488993	-0.24108750361456
C	-0.76144983225822	-4.73589834809663	-0.42279974595311
H	-3.72989242921630	-4.75812633622722	-1.84871845348840
C	-2.02305825707960	-4.30679760667946	-0.62489328650867

H	-3.04867391971966	-6.16173451553776	-0.98951398979529
H	4.34980409684171	2.49318236765426	-0.90752811140385
C	-3.25967712209937	-5.08744213883822	-0.90873517441093
H	-4.00823847856402	-4.94759552289076	-0.11273611019233
H	1.88267846206462	-4.54564522574211	0.03330904072447
C	-0.23941842730710	-6.13733348658773	-0.38407986738650
H	0.60588369699429	-6.06343694230544	1.63139363993291
H	-1.05351280356838	-6.69361894186630	1.56020581771643
H	0.30802759353537	-7.70946227689149	1.02449467564469
O	4.29606041370944	2.81299028641822	2.05043367414363
C	-0.08464625679062	-6.68188803628124	1.03895519709926
H	-0.91896657948544	-6.79076053066779	-0.95113343116323
H	0.73157974787198	-6.18412700192129	-0.90180406391840
C	-5.64460258476917	-0.13608422517684	-0.69531137494259
H	1.06665988967013	-0.74993933849216	0.00459180647654
H	-4.06708765912241	-2.53564897624379	-0.82249444470633
C	-6.05586453397910	-0.91652597309075	-1.69531358486710
C	4.44357728535812	1.73799395671146	-0.11240671584373
H	-0.27861559573019	3.35233778829088	-1.97638571132287
C	-4.57885570057322	2.77554440798954	0.10676833513864
H	-4.93476203367609	2.92231131970978	1.14031042542168
H	0.67209448447133	3.59553151422931	-3.43072314118187
C	-1.49995419293839	2.43092252153069	0.48493956786954
H	-0.39483311333586	5.04664547572214	-0.63579083765609
H	-1.12814115201930	-0.35269692515801	0.02081854478682
C	-0.11341288326509	2.40033517877213	0.47395983791090
C	0.71453270355754	1.62645163107561	-2.72380005066858
H	-5.51906082748585	-0.26671598740238	1.85586821913653
C	1.41474801864107	-3.56360683838399	0.01415038541740
C	3.13155240160119	1.02576199413591	0.09079802058530
C	6.80802917027440	3.64265518276076	1.96396094821409
C	4.22247765902945	-1.29920804247288	0.42914327481186
O	6.23969678817699	2.81691613832252	0.95098554255358
C	2.30293207499236	-2.47369809508825	0.16711208649371
H	7.86344953003378	3.77019944016285	1.70070547919724
H	6.30248140813395	4.61815426903713	1.99036715310139
N	0.68710780174865	1.32384281426190	0.25826403950818
C	1.95611044844557	1.78007103935837	0.07194308087907
C	-0.61886886288009	-0.26739217792903	-3.13518521841668
C	0.70583351059241	3.65961161279609	0.65529573376467
H	5.23218421737157	1.07117789064495	-0.47729515979310
H	-1.96360841074479	3.39683361612125	0.67199691572569
H	1.88796768930684	4.73284457772126	-1.73444231307948
H	-0.73647018346637	5.21922250344911	1.09838991875791
N	1.99719317862615	-1.14897840716764	0.13628584865943
C	0.05338344931042	4.99995777305524	0.36602636653226
C	3.72202755600351	-2.58725147999543	0.35181510593287
H	5.50999050895251	-3.73407649626013	0.65879315880469
H	4.01840113217698	-4.49229100812981	1.29142945897839
H	2.84779588251710	3.75437771084843	0.25819024258854
C	3.12602807412392	-0.37618126258940	0.25499657939012
C	0.68339079512955	3.10692593336854	-2.44171315528072
H	-1.68303283690673	-0.46265832206443	-3.30763420234146
C	5.63263496964298	-1.03056441464266	0.78454124044537
H	6.98611930384017	0.79712306978095	3.07808077073481
C	4.44126319895436	-3.88588066224940	0.47605731006543
H	4.33550614049674	-4.47320182433482	-0.44953714967679
H	6.71625873019444	3.16893390060549	2.95039649846801
H	7.53481203835392	-0.84293175025456	2.58034193023422
H	7.70479751282791	0.53605950200235	1.44895682095851
O	-0.51327577782820	1.12284156875248	-2.83788311745621
O	5.75730382357185	-0.13372373118079	1.76533577881165
H	2.79853763269395	3.28584761884332	-2.15097567043142
O	6.57827526415932	-1.61297158012021	0.30874289651586
H	-5.33743350962268	-1.27224087571341	-2.43363058872782
H	-7.09752503575171	-1.22572178936111	-1.79646209123085
C	-7.76828918802033	0.96672664082089	-0.23491894165926
C	-8.73945677665467	1.42299506726044	0.63313949481461
C	-8.55115043980496	1.27172148712004	2.00398944605196

C	-7.38753788319275	0.66315087639633	2.47012722029017
C	-6.44851771604540	0.22129270441392	1.56235088733847
N	-6.65226305614429	0.37199862628382	0.23600649242368
H	-7.83914559154061	1.07611893712835	-1.31666687932233
H	-9.62970750032780	1.90401733476791	0.22789912904377
H	-9.30515832679382	1.63022909926401	2.70712426765590
H	-7.20319011393991	0.52400217849730	3.53532836276005

S3.8) Cuarto estado triplete optimizado, T₂

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Coordinates from ORCA-job opt

C	-4.29719819215479	0.28663009005557	-0.40765847151790
C	-3.82963100492091	1.53970568648293	-0.09316461069596
N	-2.05391772945396	0.12965382364441	-0.15560522211477
C	1.97337276474417	3.32582630562493	-0.23686819526354
H	0.77899074803420	5.87645892756390	0.17833003124956
C	-2.38938604944331	1.43556129060887	0.05845664342540
H	-4.06607993017703	3.64729065093263	-0.41552372202423
H	-5.58898837351562	2.74126409833543	-0.41092768431311
C	-3.16698894642557	-0.62963666427108	-0.42635197651029
C	1.99129866870136	3.64388330678202	-1.74771073723205
H	0.94879837855998	3.79332782304882	1.56289753188812
C	0.00688745174669	-3.51852886926229	-0.24440953023700
H	-0.03946256654135	-0.89023169401079	-2.31381418250607
C	-3.16709023212852	-1.99137173645490	-0.59939586717153
C	7.02476058786980	0.04007723573257	2.33008533835153
C	4.87813274459985	2.47717709338646	1.21850986230819
C	-2.02709861100307	-2.83901372686883	-0.51622983728375
O	1.90325512984878	0.95056412314758	-2.95411261326621
H	0.15915365266400	-0.59495756611724	-4.07228889733203
N	-0.76177696147577	-2.39908088301142	-0.28757690385517
C	-0.78523176979581	-4.71489667602411	-0.45717832833591
H	-3.85684892160304	-4.73924995665295	-1.76919078705123
C	-2.07956478984373	-4.27884499332154	-0.63067594536320
H	-3.07602054939735	-6.14640347124988	-1.01803420435220
H	4.37861141224600	2.51953017983937	-0.81582110015407
C	-3.31487902411952	-5.08402617894197	-0.87427462339011
H	-4.01953080906584	-5.01612497605095	-0.02924303852257
H	1.88471862180189	-4.50723073747724	-0.00769126695825
C	-0.27263157893267	-6.12244528582513	-0.43229997656754
H	0.57580802434770	-6.08755415935541	1.58059629993783
H	-1.09129456645612	-6.69458459047604	1.50585729086882
H	0.25538439057802	-7.72367711773896	0.95704296508334
O	4.16590560291011	2.78339962489427	2.14202757281338
C	-0.12363256997136	-6.69069815060911	0.98187183048436
H	-0.95358209198637	-6.76615771367650	-1.00985622073316
H	0.69976318003595	-6.17462568372463	-0.94804914016012
C	-5.68558200463241	-0.11574893360275	-0.65361901689248
H	1.03276999973795	-0.72401998341572	-0.02336543647214
H	-4.12998196554867	-2.46770704918844	-0.78039471812267
C	-6.12449215498216	-0.86227336369872	-1.66642089511458
C	4.43316277900262	1.75165790108838	-0.02994826477182
H	-0.14408168347688	3.34511873660830	-2.18973734606065
C	-4.59813458399368	2.80881777315027	0.05512806174578
H	-4.73652521694505	3.06724290430223	1.11776272804263
H	0.89469463608149	3.54610403725111	-3.59146945081026
C	-1.53079467081401	2.48736095896256	0.32475021377342
H	-0.35767374308735	5.05971810323724	-0.91857441513803
H	-1.12524715640176	-0.28270447153878	-0.08438804524057
C	-0.12859766791540	2.47290940426519	0.33467700597545
C	0.89349408253838	1.60016410068100	-2.82506860584260
H	-5.38608329873350	-0.31368656034948	1.87936051490195
C	1.40661166059055	-3.52867272278425	-0.03156336054998
C	3.10847961387650	1.04349717068612	0.09772470349360
C	6.68235370842598	3.59840463697131	2.21910054482119
C	4.18506943122622	-1.28256843379659	0.42774551891918
O	6.16674562462579	2.80768483515656	1.15101815526442
C	2.26081976471271	-2.45581101711114	0.13349742140094
H	7.74994755988691	3.73227754103698	2.01485954711202

H	6.17623666359896	4.57331062254469	2.25239726322484
N	0.66669456104658	1.40003358604654	0.18290414692949
C	1.94812903380681	1.83289894813575	0.03092165062678
C	-0.41459627784402	-0.32279627711322	-3.17604054756699
C	0.68351272044748	3.74225829827815	0.49038483896512
H	5.23827677391537	1.09008805958427	-0.36482109928724
H	-2.00479208969517	3.45545271545089	0.47565183047078
H	2.00464283054486	4.73743786297441	-1.86069075140512
H	-0.78518081911375	5.31256255175131	0.78601955812325
N	1.95828105735984	-1.12097439811287	0.11802166274296
C	0.04131266721979	5.06409312283007	0.10494061903328
C	3.69257260703695	-2.56222018073568	0.33491340481232
H	5.48453130779955	-3.70522049566784	0.63881671019391
H	3.99529296658457	-4.46593837347343	1.27404017877510
H	2.84050061911655	3.81451080266753	0.21782822614043
C	3.09047991955987	-0.34856373765456	0.25002664189609
C	0.84399752409008	3.08827020653592	-2.58908656666379
H	-1.47797715952403	-0.54247621934655	-3.32202025770704
C	5.59457320422815	-1.01920125962487	0.80192824529482
H	6.91501477568303	0.68897817230523	3.20472648701076
C	4.41552100709588	-3.85829928155391	0.45806013878473
H	4.30867074406735	-4.44577973732431	-0.46729280840781
H	6.53944530892432	3.09101954538967	3.18253919203300
H	7.48757238196937	-0.91319173890940	2.61755486645952
H	7.64266048181981	0.52997726590227	1.56654364443732
O	-0.32793080010523	1.07768017961297	-2.92804306260463
O	5.70348998467919	-0.18245340626656	1.83549130255841
H	2.93640373102116	3.27827110606349	-2.17576889251860
O	6.54747657833448	-1.55864109655666	0.29303004601543
H	-5.43146368048824	-1.16997250680670	-2.44966156769321
H	-7.16422363728758	-1.18663031179144	-1.73834037783416
C	-7.80977935895931	0.89588665660186	-0.02511474435200
C	-8.73202912200247	1.30028347930514	0.91831301910549
C	-8.44405578831816	1.12618053174730	2.26914346813124
C	-7.23300663994711	0.54523799940227	2.63977940773629
C	-6.34589896199141	0.15394871311054	1.65972077648248
N	-6.64448730957200	0.32947964990275	0.35366562905133
H	-7.95841967864340	1.02807390879182	-1.09619183032289
H	-9.66297419892393	1.76008998252045	0.58653286594953
H	-9.15800984397350	1.44488711333413	3.03086525675311
H	-6.97112988801164	0.38791294327847	3.68612828469231

B. Energías absolutas calculadas en los puntos estacionarios

En esta sección se muestran en una tabla las energías absolutas y relativas obtenidas de los cálculos puntuales de energía usando CAM-B3LYP/def2-SVP en cada uno de las geometrías estacionarias mostradas en [Sección A](#) para el TMEe6, ZnTMEe6 y PyrTMEe6.

Tabla S1 Energías absolutas y relativas calculadas en cada punto estacionario para cada estado excitado del TMEe6

	@S0	@S1	@S2	@S3	@T1	@T2	@T3	@T4
S0 SCF (Eh)	-2103.044950	-2103.042368	-2103.040240	-2103.043639	-2103.034976	-2103.038889	-2103.042906	-2103.04201
D3BJ (Eh)	-0.114683139	-0.114780812	-0.114613627	-0.114571791	-0.114706618	-0.114984518	-0.114600037	-0.114117246
Evib (Eh)	0.74043317	0.73923845	0.73957363	0.73800981	0.73952102	0.74527704	0.74142664	0.73999715
SCF+ZPE+D3BJ	-2102.41920	-2102.417911	-2102.415280	-2102.420201	-2102.410162	-2102.408597	-2102.416079	-2102.416137
S0 Adiabatic (eV)	0	0.070	0.128	0.036	0.271	0.165	0.056	0.080
S0 ZPE+D3BJ (eV)	0	0.035	0.107	-0.027	0.246	0.289	0.085	0.083
Energías relativas de los estados excitados, full-TDDFT								
S1	2.067	1.83	1.861	1.933	1.766	1.777	1.965	1.997
S2	2.49	2.338	2.218	2.411	2.339	2.306	2.432	2.421
S3	3.149	3.084	3.195	3.015	3.097	3.114	3.024	3.007
T1	0.919	0.665	0.257	0.929	0.93	0.552	0.988	0.929
T2	1.432	0.989	1.044	1.16	1.803	0.865	1.213	1.274
T3	2.032	2.037	2.19	1.929	2.336	2.077	1.895	1.899
T4	2.474	2.478	2.417	2.364	3.037	2.552	2.351	2.268
Energías relativas de los estados excitados, TDA/TDDFT								
S1	2.226	2.022	2.047	2.106	1.973	1.979	2.134	2.161
S2	2.626	2.496	2.405	2.550	2.497	2.472	2.567	2.557
S3	3.454	3.414	3.450	3.350	3.378	3.445	3.364	3.330
T1	1.538	1.343	1.339	1.494	1.007	1.253	1.534	1.587
T2	1.763	1.546	1.374	1.700	1.715	1.498	1.779	1.725
T3	2.191	2.161	2.354	2.021	2.223	2.208	1.959	1.986
T4	2.612	2.605	2.584	2.477	2.728	2.679	2.458	2.375

Tabla S2 Energías absolutas y relativas calculadas en cada punto estacionario para cada estado excitado del ZnTMEe6

	@S0	@S1	@S2	@S3	@T1	@T2	@T3	@T4
S0 SCF (Eh)	-3881.204494	-3881.200060	-3881.197112	-3881.202077	-3881.194798	-3881.193715	-3881.201648	-3881.199066
D3BJ (Eh)	-0.121276715	-0.121407567	-0.121973879	-0.121667987	-0.121802865	-0.121748013	-0.121425179	-0.121811016
Evib (Eh)	0.71784301	0.71599784	0.71767498	0.71503161	0.71680807	0.72062613	0.71742254	0.7174469
SCF+ZPE+D3BJ	-3880.607928	-3880.605470	-3880.601410	-3880.608713	-3880.599793	-3880.594837	-3880.605651	-3880.603430
S0 Adiabatic (eV)	0	0.121	0.201	0.066	0.264	0.293	0.077	0.148
S0 ZPE+D3BJ (eV)	0	0.067	0.177	-0.021	0.221	0.356	0.062	0.122
Energías relativas de los estados excitados, full-TDDFT								
S1	2.075	1.825	1.867	2.003	1.730	1.836	2.062	2.098
S2	2.556	2.362	2.202	2.463	2.384	2.133	2.529	2.483
S3	3.174	3.145	3.131	3.037	3.132	3.031	3.048	3.033
T1	1.062	0.651	0.748	0.987	0.014	0.675	1.042	1.127
T2	1.604	1.241	1.029	1.460	1.459	0.858	1.592	1.509
T3	2.107	2.126	2.157	1.950	2.190	2.105	1.901	1.929
T4	2.511	2.342	2.285	2.444	2.427	2.342	2.445	2.321
Energías relativas de los estados excitados, TDA/TDDFT								
S1	2.235	2.017	2.049	2.169	1.931	2.022	2.221	2.249
S2	2.680	2.511	2.369	2.588	2.526	2.317	2.645	2.603
S3	3.443	3.330	3.217	3.327	3.241	3.114	3.345	3.320
T1	1.486	1.197	1.262	1.440	1.021	1.235	1.497	1.566
T2	1.919	1.703	1.486	1.878	1.764	1.358	1.962	1.900
T3	2.295	2.283	2.379	2.105	2.288	2.343	2.078	2.099
T4	2.730	2.578	2.483	2.584	2.509	2.515	2.578	2.451

Tabla S3 Energías absolutas y relativas calculadas en cada punto estacionario para cada estado excitado del PyrTMEe6

	@S0	@S1	@S2	@S3	@S4	@T1	@T2	@T3	@T4
S0 SCF (Eh)	-2350.26037	-2350.2583	-2350.255913	-2350.251396	-2350.259272	-2350.251136	-2350.254854	-2350.258055	-2350.257738
D3BJ (Eh)	-0.129925678	-0.130141497	-0.129958646	-0.130029427	-0.129936436	-0.129935355	-0.130433296	-0.129854005	-0.129468822
Evib (Eh)	0.82313359	0.82262033	0.8225575	0.82150026	0.8234816	0.82266897	0.82839841	0.82437681	0.82355148
SCF+ZPE+D3BJ	-2349.567163	-2349.565915	-2349.563314	-2349.559925	-2349.565726	-2349.558402	-2349.556889	-2349.563533	-2349.563655
S0 Adiabatic (eV)	0	0.054	0.121	0.244	0.030	0.251	0.150	0.063	0.072
S0 ZPE+D3BJ (eV)	0	0.034	0.105	0.197	0.039	0.238	0.280	0.099	0.095
Energías relativas de los estados excitados, <i>full</i>-TDDFT									
S1	1.921	1.812	1.818	1.925	1.909	1.745	1.758	1.933	1.954
S2	2.408	2.320	2.190	2.426	2.408	2.263	2.286	2.419	2.398
S3	3.027	3.042	3.151	2.426	2.963	2.999	3.034	2.989	2.993
S4	3.105	3.122	3.237	3.075	3.034	3.093	3.139	3.054	3.085
T1	0.831	0.569	0.191	0.875	0.872	0.876	0.436	0.939	0.841
T2	1.141	0.964	1.026	1.138	1.122	1.702	0.840	1.171	1.203
T3	2.026	2.054	2.248	1.984	1.942	2.337	2.095	1.889	1.918
T4	2.446	2.489	2.502	2.405	2.386	3.000	2.558	2.358	2.284
Energías relativas de los estados excitados, TDA/TDDFT									
S1	2.103	2.009	2.015	2.109	2.090	1.960	1.966	2.109	2.127
S2	2.557	2.483	2.385	2.430	2.549	2.429	2.456	2.555	2.539
S3	3.046	3.073	3.203	2.566	2.972	3.019	3.053	3.031	3.084
S4	3.410	3.413	3.437	3.188	3.357	3.385	3.443	3.349	3.317
T1	1.448	1.316	1.288	1.429	1.458	0.997	1.232	1.499	1.531
T2	1.634	1.511	1.329	1.727	1.682	1.642	1.458	1.756	1.659
T3	2.149	2.182	2.354	2.067	2.036	2.224	2.229	1.953	2.024
T4	2.559	2.608	2.572	2.414	2.495	2.788	2.680	2.464	2.386

C. Estructura electrónica en la geometría optimizada del estado basal

En la [Tabla S4](#) y [S5](#) se muestra la estructura electrónica de los estados excitados calculada sobre de los mínimos encontrados en la optimización del estado fundamental (S_0) usando *full*-TDDFT(CPCM)/def2-SVP y TDA/TDDFT(CPCM)/def2-SVP.

Tabla S4 Caracterización de estados excitados en la geometría del estado basal del trimetil éster de clorina e6 y sus derivados con zinc y piridina en CH₂Cl₂. Calculados con *full*-TDDFT/CAM-B3LYP(CPCM)/def2-SVP

Molécula	Estado	VEEs (eV)[f_{osc}]	λ (nm)	$ \mu ^2$ (a.u.) ²	Contribuciones
TMEe6	S1(Qy)	2.067 [0.423]	600	8.35	HOMO→LUMO:0.85
	S2(Qx)	2.490 [0.145]	498	2.37	HOMO-1→LUMO:0.70, HOMO→LUMO+1:0.24
	S3(By)	3.149 [1.663]	394	21.56	HOMO→LUMO+1:0.72, HOMO-1→LUMO:0.25
	S4(Bx)	3.308 [1.510]	375	18.63	HOMO-1→LUMO+1:0.83
	T1	0.919	-	-	HOMO→LUMO:0.92
	T2	1.432	-	-	HOMO-1→LUMO:0.91
	T3	2.032	-	-	HOMO→LUMO+1:0.68, HOMO-1→LUMO:0.28
	T4	2.472	-	-	HOMO-1→LUMO+1:0.83
ZnTMEe6	S1(Qy)	2.075 [0.519]	598	10.21	HOMO→LUMO:0.91
	S2(Qx)	2.556 [0.139]	485	2.22	HOMO-1→LUMO:0.75, HOMO→LUMO+1:0.20
	S3(By)	3.174 [1.513]	390	19.45	HOMO→LUMO+1:0.76, HOMO-1→LUMO:0.20
	S4(Bx)	3.480 [1.324]	356	15.53	HOMO-1→LUMO+1:0.75, HOMO-2→LUMO:0.12
	S5(n)	3.548 [0.142]	349	1.63	HOMO-2→LUMO:0.67, HOMO-1→LUMO+1:0.12
	S6(σ)	3.640 [0.032]	340	0.36	HOMO-4→LUMO:0.73, HOMO-5→LUMO:0.20
	T1	1.062	-	-	HOMO→LUMO:0.80
	T2	1.604	-	-	HOMO-1→LUMO:0.76, HOMO→LUMO:0.10
PyrTMEe6	T3	2.107	-	-	HOMO→LUMO+1:0.82
	T4	2.511	-	-	HOMO-2→LUMO:0.52, HOMO-2→LUMO+1:0.10
	S1(Qy)	1.921 [0.439]	645	9.33	HOMO→LUMO:0.88
	S2(Qx)	2.408 [0.095]	515	1.62	HOMO-1→LUMO:0.72, HOMO→LUMO+2:0.25
	S3(CT)	3.027 [0.333]	410	4.50	HOMO→LUMO+1:0.75, HOMO→LUMO+2:0.13
	S4(By)	3.105 [1.300]	399	17.10	HOMO→LUMO+2:0.58, HOMO→LUMO+1:0.19, HOMO-1→LUMO:0.18
	S5(Bx)	3.258 [1.407]	381	17.63	HOMO→LUMO+2:0.81
	T1	0.831	-	-	HOMO-1→LUMO:0.66, HOMO→LUMO+2:0.17
	T2	1.141	-	-	HOMO→LUMO:0.86,
	T3	2.026	-	-	HOMO→LUMO+2:0.74, HOMO-1→LUMO:0.19
	T4	2.446	-	-	HOMO-1→LUMO+2:0.86

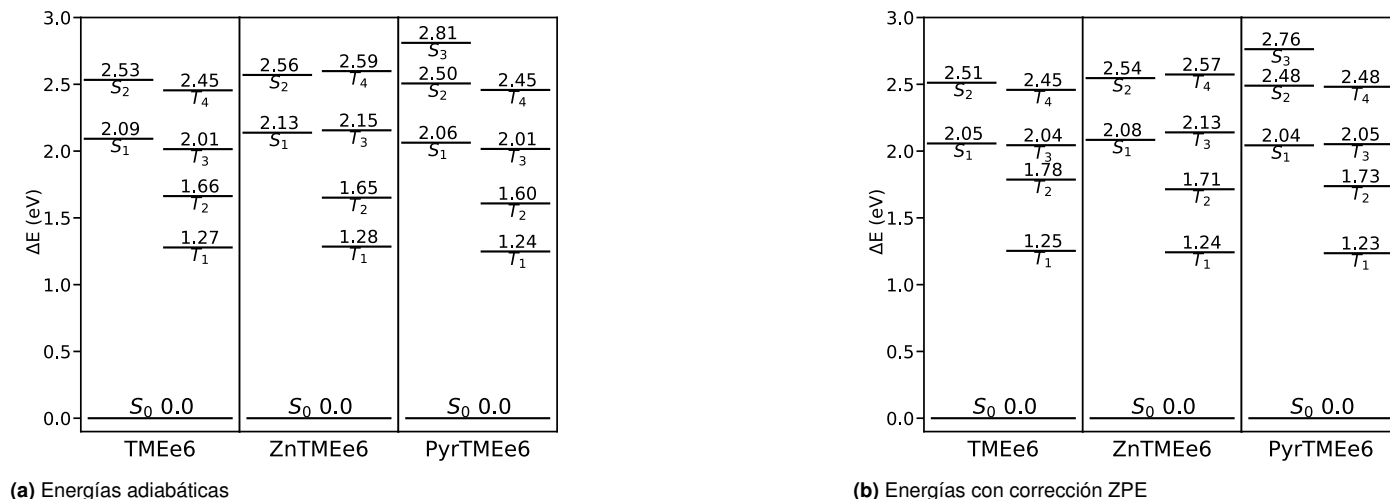
Tabla S5 Caracterización de estados excitados en la geometría del estado basal del trimetil éster de clorina e6 y sus derivados con zinc y piridina en CH₂Cl₂. Calculados con TDA-TDDFT/CAM-B3LYP(CPCM)/def2-SVP

Molécula	Estado	VEEs (eV)[f_{osc}]	λ (nm)	$ \mu ^2$ (a.u.) ²	Contribuciones
TMEe6	S1(Qy)	2.226 [0.466]	557	8.54	HOMO→LUMO:0.80, HOMO-1→LUMO+1:0.12
	S2(Qx)	2.626 [0.121]	472	1.88	HOMO-1→LUMO:0.64, HOMO→LUMO+1:0.29
	S3(By)	3.454 [2.429]	359	28.70	HOMO→LUMO+1:0.66, HOMO-1→LUMO:0.28
	S4(Bx)	3.516 [2.137]	353	24.80	HOMO-1→LUMO+1:0.76, HOMO→LUMO:0.12
	T1	1.538	-	-	HOMO→LUMO:0.70, HOMO-1→LUMO:0.20
	T2	1.763	-	-	HOMO-1→LUMO:0.70, HOMO→LUMO:0.23
	T3	2.191	-	-	HOMO→LUMO+1:0.88
	T4	2.612	-	-	HOMO-1→LUMO+1:0.87
ZnTMEe6	S1(Qy)	2.235 [0.592]	555	10.81	HOMO→LUMO:0.87
	S2(Qx)	2.680 [0.114]	463	1.75	HOMO-1→LUMO:0.68, HOMO→LUMO+1:0.27
	S3(By)	3.443 [1.977]	360	23.44	HOMO→LUMO+1:0.67, HOMO-1→LUMO:0.23
	S4(n)	3.610 [0.758]	343	8.57	HOMO-2→LUMO:0.60, HOMO-1→LUMO+1:0.18
	S5(σ)	3.658 [0.097]	339	1.08	HOMO-4→LUMO:0.64, HOMO-5→LUMO:0.23
	S6(Bx)	3.706 [1.454]	334	16.01	HOMO-1→LUMO+1:0.62, HOMO-2→LUMO:0.11
	T1	1.486	-	-	HOMO→LUMO:0.90
	T2	1.919	-	-	HOMO-1→LUMO:0.91
	T3	2.295	-	-	HOMO→LUMO+1:0.90
	T4	2.730	-	-	HOMO-1→LUMO+1:0.79
PyrTMEe6	S1(Qy)	2.103 [0.485]	589	9.33	HOMO→LUMO:0.82, HOMO-1→LUMO+2:0.14
	S2(Qx)	2.557 [0.072]	485	1.62	HOMO-1→LUMO:0.64, HOMO→LUMO+2:0.32
	S3(CT)	3.046 [0.013]	407	0.18	HOMO→LUMO+1:0.95
	S4(By)	3.105 [2.284]	364	27.34	HOMO→LUMO+2:0.59
	S5(Bx)	3.258 [1.846]	356	21.63	HOMO-1→LUMO+2:0.63, HOMO→LUMO:0.11
	T1	1.448	-	-	HOMO→LUMO:0.95
	T2	1.634	-	-	HOMO-1→LUMO:0.89
	T3	2.149	-	-	HOMO→LUMO+2:0.90
	T4	2.559	-	-	HOMO-1→LUMO+2:0.90

D. Diagramas de energías

Usando las energías calculadas con TDA de [Tabla S1](#), [Tabla S2](#) and [Tabla S3](#), se realizaron dos diagramas de energías en [Figura S1](#), que muestran de manera resumida las energías relativas de las estructuras optimizadas de los estados excitados respecto a la energía del estado basal. Se hace la distinción entre energías adiabáticas, y energías con corrección vibracional del punto cero (ZPE).

Figura S1 Diagramas de energías relativas de los estados excitados respecto al estado basal en sus geometrías de equilibrio



Se añaden también diagramas de energías más generales ([Figura S2-Figura S7](#)), en donde se incluyen todas las energías relativas de los estados excitados en cada geometría de equilibrio. La energía del estado excitado optimizado en cuestión se muestra en negrilla.

Figura S2 Diagrama de energías adiabáticas en cada geometría estacionaria para el TMEe6

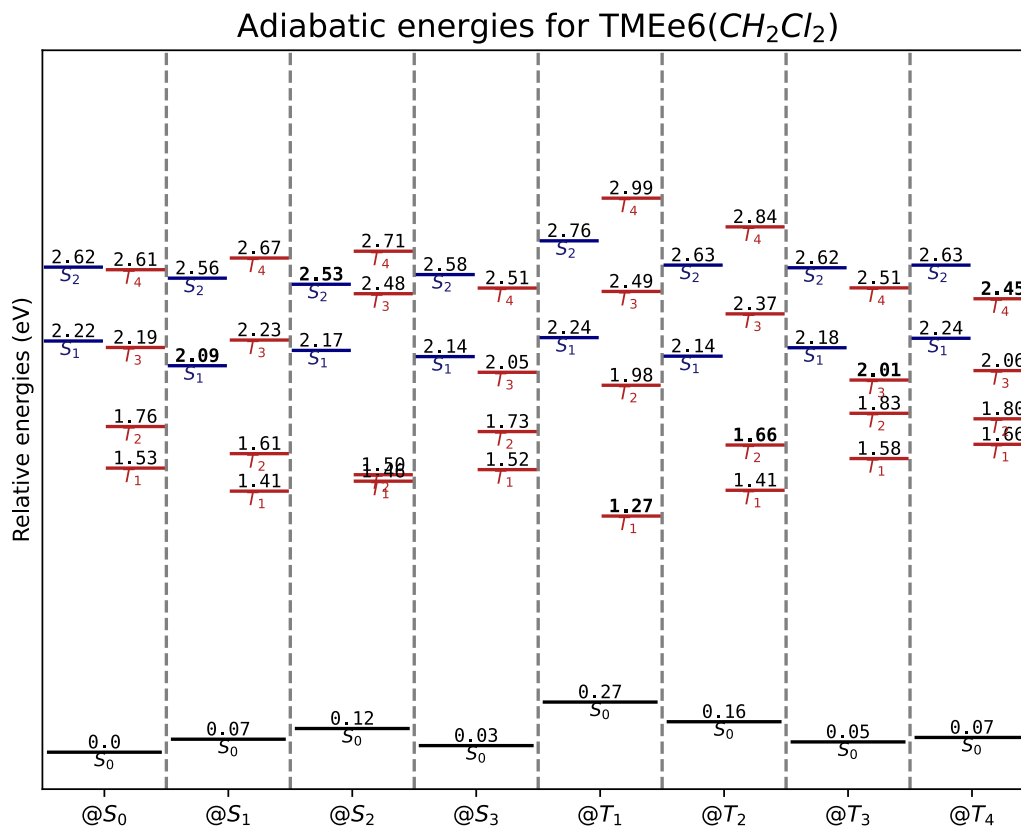


Figura S3 Diagrama de energías adiabáticas en cada geometría estacionaria para el ZnTMEe6

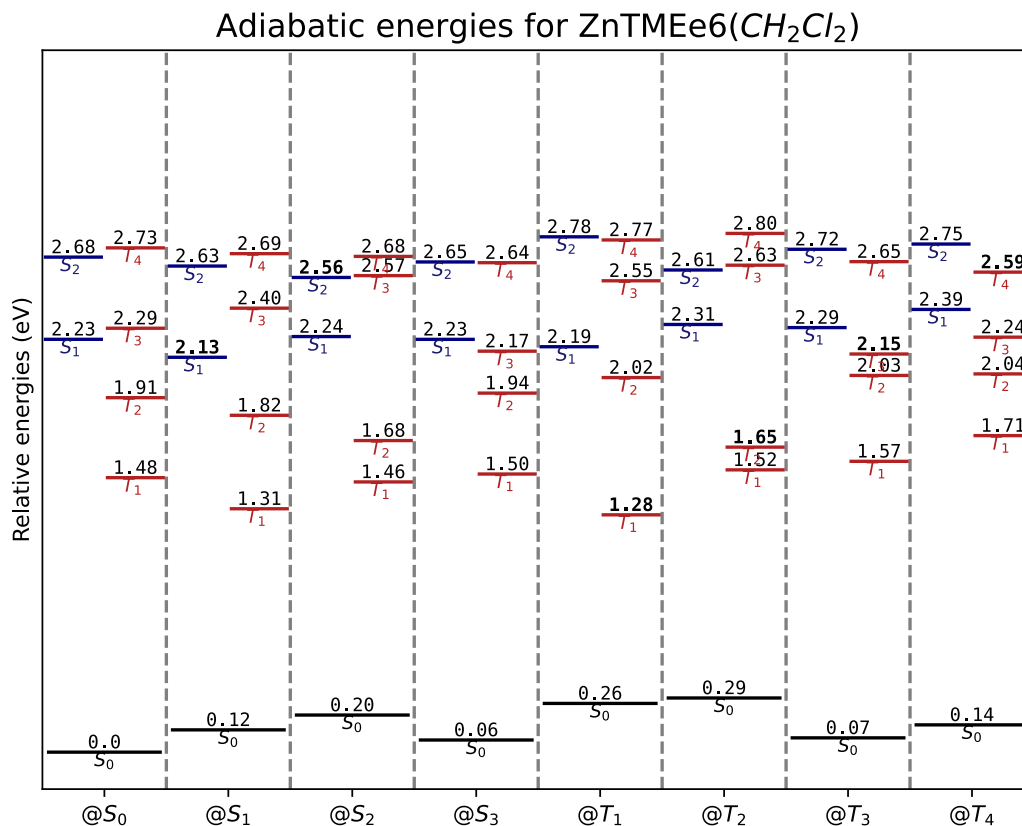


Figura S4 Diagrama de energías adiabáticas en cada geometría estacionaria para el PyrTMEe6

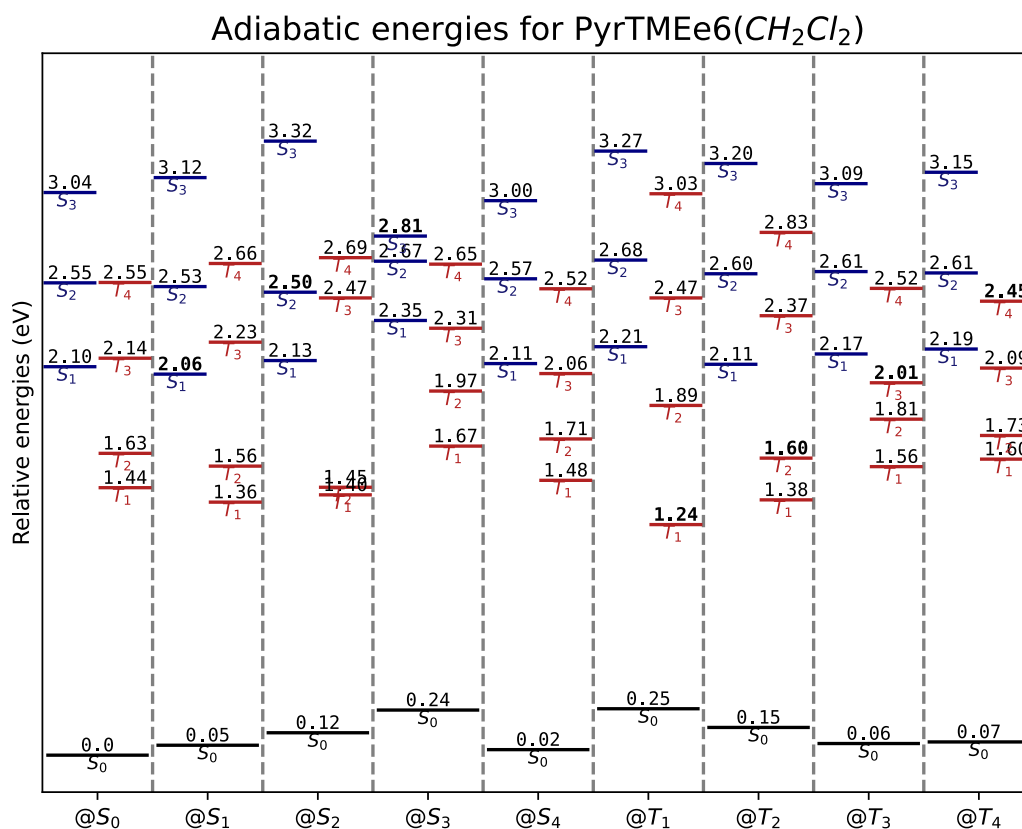


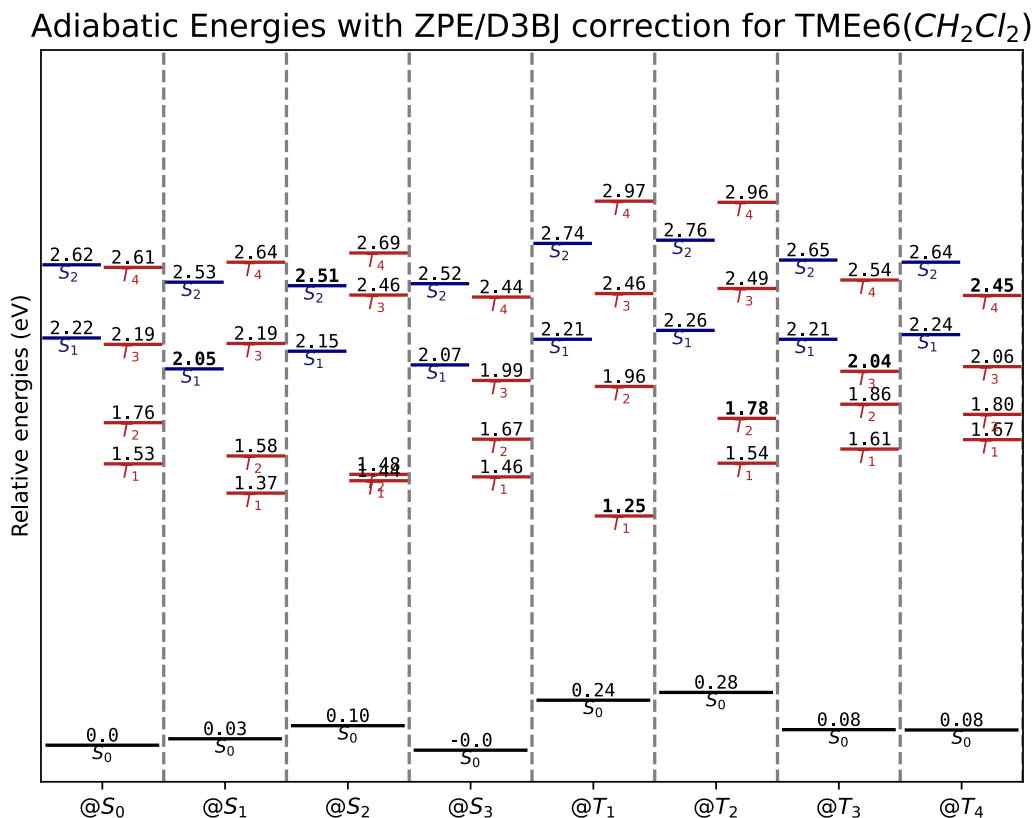
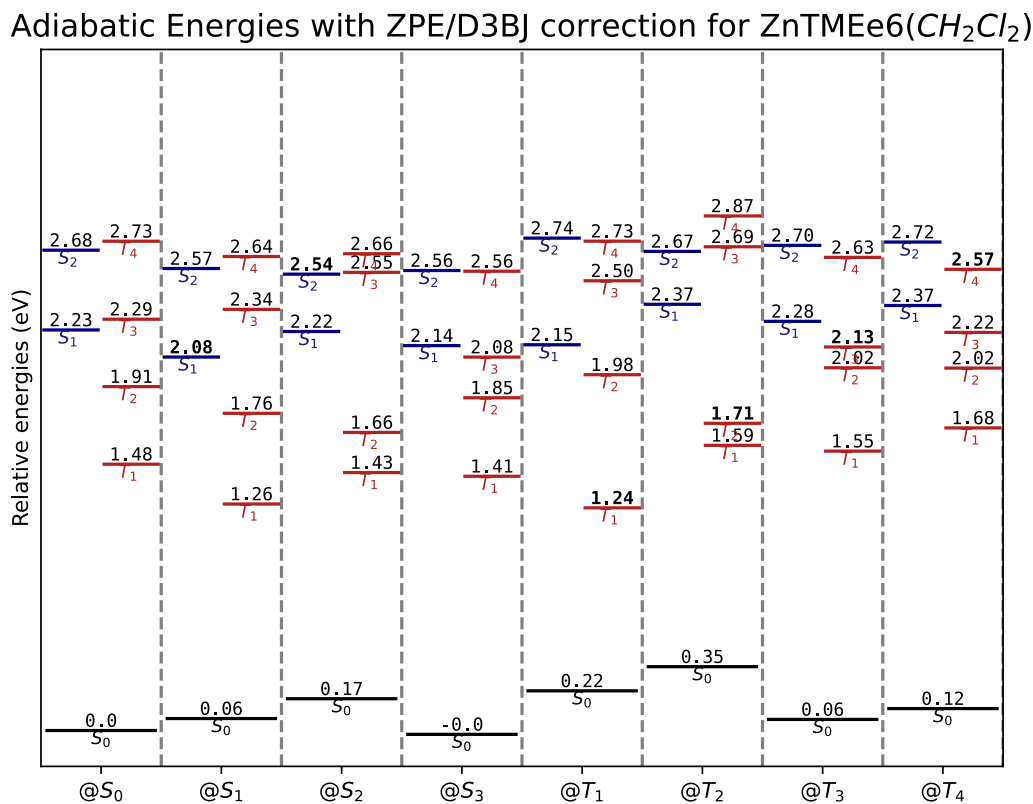
Figura S5 Diagrama de energías con corrección ZPE en cada geometría estacionaria para el TMEe6**Figura S6** Diagrama de energías con corrección ZPE en cada geometría estacionaria para el ZnTMEe6

Figura S7 Diagrama de energías con corrección ZPE en cada geometría estacionaria para el PyrTMEe6Adiabatic Energies with ZPE/D3BJ correction for PyrTMEe6(CH_2Cl_2)