

Stabilization of TADF emitters by suppressing charge-induced C–N bond cleavage**Nikita O. Dubinets and Andrey Yu. Sosorev**

Table S1. Total energy and atomic coordinates for Cz-TRZ molecule.

E= -1489.590073520616

N	-3.95770226058293	0.00307195145268	-0.03366368978396
N	2.37978208002777	1.14812673912148	0.29316010339961
N	2.38270996095344	-1.15037300169420	-0.25222311082822
N	4.42554927738569	-0.00269520006774	0.03797467552754
C	-4.76966334196173	0.95496209365475	-0.66478315370089
C	-4.78168733239423	-0.94850065072800	0.58212576352538
C	-6.13229012713525	0.61010216630582	-0.45165955181923
C	-6.13995315225790	-0.60283316617933	0.34397990485210
C	-2.54644749129412	0.00219153397819	-0.02161351092546
C	-4.41113013340625	2.06399575701768	-1.43984204513176
C	-4.43812741763419	-2.05809627454805	1.36316712240073
C	-7.14450807789797	1.40711517747668	-1.00288465721708
C	-7.16256996588814	-1.39948379873831	0.87623084067418
C	-1.83979242004457	1.16126261556392	0.33969600128804
C	-1.83522383658817	-1.15771181594846	-0.37103860524553
C	-5.43828539771561	2.84162707162977	-1.97920774435365
C	-5.47543554686278	-2.83539041595284	1.88321242850245
C	-6.79229689078361	2.52428665537002	-1.76049592004285
C	-6.82498647724955	-2.51713425473368	1.63975747262599
C	0.26938171037273	0.00041421037555	0.00224825309511
C	-0.44774931485461	1.16057948537873	0.34127140570847
C	-0.44337719734822	-1.15882738564572	-0.34900895849673
C	1.75010254438381	-0.00065095324315	0.01503378259653
C	3.71873422875669	1.10626803605140	0.29184512138432
C	3.72149134478105	-1.11058345704186	-0.22794117827067
C	4.45906956815950	2.35680801102818	0.58526419376489
C	4.46474525367896	-2.36238801805658	-0.50829322107974
C	5.86460656368068	2.36312757987693	0.59959081962699
C	3.76321226085919	3.54918380839635	0.84936051837279
C	5.87033062754000	-2.37045507791214	-0.50106704760774
C	3.77152427544534	-3.55423823038450	-0.78153190487738
C	6.56057953235213	3.54084548357071	0.87311489975896
C	4.46145840852788	4.72567344213467	1.12231867007579
C	6.56893126750073	-3.54931515317244	-0.76271186703552
C	4.47238309303427	-4.73190949452493	-1.04236540687699
C	5.86114542842078	4.72465274875900	1.13491117357822
C	5.87209757711514	-4.73258071580401	-1.03373346481742
H	-3.36475130894106	2.31266028881792	-1.62695405249240
H	-3.39551760372306	-2.30754005424841	1.56932870260635
H	-8.19633886492239	1.15158932848601	-0.84333850841421
H	-8.21116908213298	-1.14337832291444	0.69747453370677
H	-2.39173655175994	2.05603468303724	0.63572733462860
H	-2.38322846012369	-2.05175437450509	-0.67642160545494
H	-5.18096150569208	3.71438625246386	-2.58723536668203
H	-5.22981854863218	-3.70857230530967	2.49545613096388
H	-7.57232351596769	3.15640634988956	-2.19482027477040
H	-7.61324435464074	-3.14898072170660	2.05936872138590

H	0.10691973457984	2.05717301996603	0.62341004998030
H	0.11485115866555	-2.05609786084029	-0.62182772632360
H	6.39550046113886	1.43206168431692	0.39318349008671
H	2.67193500993836	3.53430766100496	0.83536501714772
H	6.39911501036177	-1.43981306220901	-0.28748520149520
H	2.68018197515768	-3.53797783284093	-0.78412068884276
H	7.65482811811827	3.53737271337304	0.88246642655323
H	3.91253961601057	5.65005245731155	1.32654093311086
H	7.66319949821465	-3.54722825496412	-0.75548287967021
H	3.92549481888096	-5.65589759729124	-1.25368164477139
H	6.40790118267349	5.64841668712929	1.34911683467304
H	6.42091459171985	-5.65724824173313	-1.23856833857347

Table S2. Total energy and atomic coordinates for (1) mCz-TRZ molecule.

E= -1489.593492485818

N	-3.17819373618094	-0.90626691978589	-0.58762587973599
N	2.33188117359680	1.44733609486797	0.47601325132203
N	1.84071224737277	-0.76204456638544	-0.18343009469807
N	4.07617907102340	-0.11212057837051	0.18255011054575
C	-4.20382160124818	-0.78138266585690	-1.52528575467717
C	-3.23501026904562	-2.18624689508208	-0.03273870804318
C	-4.92894985891093	-1.99553087913646	-1.57277406793216
C	-4.31220331769795	-2.89051797107948	-0.62019744226631
C	-2.69958164849032	1.36556299389972	0.14405005435584
C	-4.52144188586067	0.28918090971166	-2.35520791518628
C	-2.44496927119622	-2.75857445587082	0.95954963511150
C	-6.00128851918658	-2.12177171701872	-2.45382420996391
C	-4.58401762848761	-4.19520638584614	-0.21234087021833
C	-1.78049574842635	2.34521867712062	0.49668189815543
C	-2.25169305895591	0.10003743380784	-0.23440689144124
C	-5.59407351732040	0.13687927617879	-3.22391776130301
C	-2.73781911069924	-4.05893400570449	1.34782099338275
C	-6.33180626219079	-1.05194520799468	-3.27222705006456
C	-3.79259906400873	-4.77438806745732	0.76810914850097
C	0.03127044991921	0.79933652923934	0.13044537973053
C	-0.42098319050973	2.06807407818643	0.49898149373823
C	-0.89034074185602	-0.17632512886749	-0.24997790017352
C	1.47637153811369	0.48040802752357	0.13886638413090
C	3.62506289341488	1.10797762933037	0.48562983522206
C	3.15201931370330	-1.01779704020580	-0.14939992632462
C	4.61228494744439	2.14334347635648	0.85583736877136
C	3.60228596955128	-2.38121137771684	-0.49682257165325
C	5.97524286721306	1.83671802550593	0.90101769940915
C	4.19335126050749	3.43982716411725	1.16778804935899
C	4.95860508886156	-2.71397240040313	-0.43882086747536
C	2.67602711231080	-3.35302317071126	-0.88670588537803
C	6.89963389215028	2.80809956030385	1.25476822323638
C	5.12049615920653	4.40912394189204	1.51989683235312
C	5.37904841198891	-3.99473559435423	-0.76418131648373
C	3.10039441169914	-4.63202063149051	-1.21405044322755
C	6.47528335113142	4.09609101240156	1.56565080852183
C	4.45193471946771	-4.95644107875791	-1.15333592858481
H	-3.95094976904005	1.20707458718610	-2.33507202099159
H	-1.63258413729756	-2.21274380111589	1.41783243580564
H	-6.56533327899597	-3.04479143702843	-2.50182642134001
H	-5.40533105178169	-4.74693852812855	-0.65232376533939
H	-2.13126464368840	3.32633703847296	0.78936956532935

H	-5.86142020095543	0.95587507982767	-3.87925421892542
H	-2.13649087936933	-4.52641357739301	2.11693319215278
H	-7.16299511651698	-1.13593807754731	-3.95993115315717
H	-3.99228464625022	-5.78696821803179	1.09328122776078
H	0.29990331959965	2.81870726635036	0.78666227788507
H	-0.53442167483505	-1.14744470259551	-0.55774563816890
H	6.29226914369855	0.83326735254781	0.65755016648549
H	3.13891454571802	3.67071807343392	1.12888737279296
H	5.66861595884881	-1.95813202152633	-0.13661850100486
H	1.62898094604566	-3.09118000412060	-0.92857117882781
H	7.95311127586381	2.56157919577169	1.28882122753615
H	4.78722977817827	5.41073003319619	1.75964896547788
H	6.43115577824746	-4.24457543710001	-0.71503811353748
H	2.37639145055046	-5.37766375422803	-1.51645494065136
H	7.19792745126551	4.85344373748491	1.84213743287772
H	4.78165174209863	-5.95576469165894	-1.40807284877571
H	-3.76152668478861	1.56813815585555	0.17089124060019

Table S3. Total energy and atomic coordinates for (2) oCz-TRZ molecule.

E= -1489.595539996269

N	-0.64328004794971	-2.32170463153993	-0.63788389010566
N	1.94735594156533	0.71273279788038	0.22812725824473
N	1.86143895853134	-1.14749530815266	-1.21880235603170
N	3.88840250093466	-0.56895415898091	-0.16686895522543
C	-0.57325444092463	-3.28923123522423	-1.63726972060133
C	0.03566910153370	-2.79215546401544	0.48395520729091
C	0.12206886208901	-4.41518237774627	-1.13653506955715
C	0.51702575488821	-4.09440769395556	0.21635662800502
C	-2.87183711543903	0.56604572364063	-1.22563765084807
C	-1.02173709563350	-3.23081710157228	-2.95110011484217
C	0.26669899615256	-2.16067565569627	1.70058492268364
C	0.33977124935991	-5.51095477306374	-1.96832457056795
C	1.24662094103916	-4.76859708595587	1.19348495228375
C	-1.98523746806546	1.63129829125122	-1.11430302958759
C	-2.41383487510191	-0.73477333860695	-1.06740592723262
C	-0.78425041863065	-4.33312095331286	-3.76218210633773
C	1.00278574640029	-2.85117379100260	2.65389222553748
C	-0.11734426742091	-5.46514878485419	-3.27749518590423
C	1.48900789320222	-4.14086357990639	2.40654398179274
C	-0.15863591833397	0.08366720473882	-0.75362613342155
C	-0.64270202821951	1.38768218166541	-0.86643485305046
C	-1.06550122662416	-0.98477974359175	-0.83271791925295
C	1.29679485432116	-0.13201546023277	-0.57121941953827
C	3.25184709950184	0.45872081048882	0.39826232455237
C	3.16116691022287	-1.34624322404689	-0.97516913065274
C	4.02460960836718	1.36310913187867	1.27445207426761
C	3.81489838508094	-2.49666758794244	-1.62718883169417
C	5.39735831370804	1.17099743474365	1.45347067164622
C	3.39011863649429	2.41949745072945	1.93434732863948
C	5.14649733516414	-2.81104144797991	-1.33990040098246
C	3.09933855966344	-3.29437239411028	-2.52463114026730
C	6.12119296760050	2.02145541436140	2.27567004322416
C	4.11703680005078	3.26713703313338	2.75700478915045
C	5.75013775243653	-3.90558818947424	-1.93972159513896
C	3.70723709345960	-4.38751686172615	-3.12279806678757
C	5.48358122988522	3.07123739602337	2.92950224311106
C	5.03194454031894	-4.69646288520215	-2.83216891522610

H	-1.52287787557206	-2.35233693636442	-3.33369341263829
H	-0.09912915203425	-1.16174713431512	1.89475920060222
H	0.87773246960974	-6.37677400121478	-1.60366992821214
H	1.62901238334039	-5.76361903903498	1.00370392454406
H	-2.33895981073421	2.64853354007413	-1.21934084540330
H	-1.11942895119424	-4.31308454391638	-4.79125914847355
H	1.20641677086461	-2.37928439318067	3.60644833795375
H	0.04839228941228	-6.30792847755927	-3.93589857179526
H	2.06246143646770	-4.64911160499274	3.17049297865968
H	0.05912976589441	2.20521469042153	-0.77578499813562
H	5.87993779796630	0.35205346673092	0.94031110921387
H	2.32795368043432	2.55865285764017	1.79418218511978
H	5.69045253418851	-2.19195145109200	-0.64139751401905
H	2.06928044004756	-3.05375668533076	-2.73772415589328
H	7.18432109225166	1.86633062166998	2.40790453652489
H	3.61779678254176	4.08176801405336	3.26593010515194
H	6.78065051048025	-4.14531324221002	-1.71067515451536
H	3.14051163249305	-5.00170842872751	-3.81001317673576
H	6.04980978749339	3.73391043283045	3.57180747645694
H	5.50447372824403	-5.55200350732377	-3.29851915400040
H	-3.92238503820458	0.74723414322095	-1.41243063598924
H	-3.09702237461915	-1.57270499102143	-1.10526617499129

Table S4. Total energy and atomic coordinates for (3) CF₃_Cz-TRZ molecule.

E= -1826.662147343222

N	-3.55242656809435	-0.22235400586332	0.11083155909234
N	2.71666794103328	0.88913350350136	-0.72478508588722
N	2.79998462336161	-0.99971644958224	0.68542139578563
N	4.79785014538741	0.00917237124195	-0.05252088452248
C	-5.71092248873688	-0.37979175702212	-0.61316623858435
C	-5.69197220430914	0.39842212186007	0.60637994160545
C	-4.37067269457137	-0.73155443522841	-0.89631646193885
C	-4.34092487994602	0.48804177417000	1.01497053476887
C	-2.13539141523250	-0.21403449618458	0.08722610706355
C	-6.72007593962910	-0.79585030874113	-1.47971410903367
C	-6.67603085626421	1.02420922387471	1.36939450402609
C	-4.02264544168918	-1.46957195974480	-2.02011152969885
C	-3.95829284992241	1.19131333679364	2.14985845977251
C	-6.38199816143593	-1.53737591488211	-2.60258733099521
C	-6.30318756056332	1.72681653777442	2.50634141440216
C	-5.04729436932059	-1.86693314025718	-2.86853542181909
C	-4.95859916243152	1.80987689986814	2.88812012126822
C	-1.47989199905806	0.82976964551762	-0.55641210632905
C	-1.38418166751318	-1.22492196851223	0.69892982263752
C	-0.09603922062838	0.87884550540563	-0.59670272217635
C	0.00139018533187	-1.16981892481435	0.66291962159159
C	0.65694758736991	-0.12123157966579	0.01724621498332
C	2.13763640666841	-0.07520688735274	-0.00914896108548
C	4.05507985973873	0.89161773882867	-0.72533034874998
C	4.13495763990836	-0.91890726504687	0.64274626810751
C	4.74891251133496	1.92809259370182	-1.51626268918782
C	4.91634060096913	-1.91074750522324	1.40770011734839
C	6.14573334898034	1.97695454198596	-1.54482577798173
C	4.01744270085841	2.86768007571468	-2.24861017954185
C	6.31366871127326	-1.86716369248846	1.39985953465742
C	4.26739669186355	-2.90254756736377	2.14932614365617
C	6.79646913508453	2.94775313296888	-2.29106946728163

C	4.67151905388253	3.83714772169233	-2.99381413821556
C	7.04621202728931	-2.79790518909533	2.12071015180682
C	5.00341000674415	-3.83179847510953	2.86874209751112
C	6.06194658666366	3.87978199476020	-3.01739344247920
C	6.39375027347062	-3.78248843749199	2.85622142585289
H	-7.75370516747510	-0.54202888350991	-1.28042416474504
H	-7.71700278665618	0.96488301479994	1.07724497224094
H	-2.99308523410971	-1.73221997394628	-2.22276992404971
H	-2.92106545341511	1.25046000218086	2.45127885311685
H	-4.80811569820385	-2.44651949311613	-3.75086096132194
H	-4.69187414979119	2.36463525667546	3.77850466255803
H	-2.07682581822324	1.60195237312810	-1.02280849752724
H	0.41472128456304	1.68844034410025	-1.09688224320704
H	0.59018760209896	-1.93950563296070	1.13573500923885
H	6.70522285812046	1.24753724074653	-0.97775820568529
H	2.93847179353344	2.82370857545291	-2.22522043787044
H	6.80893123938717	-1.09838138792987	0.82504062542282
H	3.18767928839805	-2.93120077580646	2.15392959926814
H	7.87835387397943	2.97810474111811	-2.30807465814304
H	4.09728727770706	4.56048813139695	-3.55839155341653
H	8.12782810554367	-2.75691637162798	2.10968865070636
H	4.49271142260605	-4.59597588225661	3.44040849213528
H	6.57154753107518	4.63659998679785	-3.60028512263992
H	6.96711994894742	-4.50862114890690	3.41855168326432
C	-2.06913015071537	-2.37284067301446	1.40191700698587
F	-2.85060626921600	-1.94945158887210	2.41460588413868
F	-2.85289456881124	-3.08362951417702	0.56664815924876
F	-1.17848101068840	-3.23749267182158	1.92954551638184
H	-7.05774459346685	2.21814166559736	3.10651409282208
H	-7.15666437205555	-1.86621048303824	-3.28282875635183

Table S5. Total energy and atomic coordinates for (4) CH₃_Cz-TRZ molecule.

E= -1528.902527176822			
N	-3.47890342542291	0.08693172204817	-0.03403739778450
N	2.83039471540950	1.00842187672270	-0.72486855136360
N	2.82225904162249	-0.91698463705105	0.63662029778638
N	4.86768106957110	0.03852372755698	-0.04228093159785
C	-4.29074313093184	-0.32100285144466	-1.08811028529825
C	-4.28671371099046	0.49337088460369	1.02191594636293
C	-5.64607502757668	-0.18062371529931	-0.70263919667529
C	-5.64340056543755	0.34197550663137	0.64618002521218
C	-2.06063004076413	0.06165646233815	-0.02907281508373
C	-6.64979070713443	-0.54510038358541	-1.59880692014908
C	-6.64368820897344	0.70046520078368	1.54858427783603
C	-3.92683513090465	-0.81947686019997	-2.33379680738111
C	-3.91884246886812	0.99832349291146	2.26389662048509
C	-1.38083873155185	-0.90498596183758	0.72397008006198
C	-6.29399950536166	-1.03807773550351	-2.84603016385505
C	-6.28354009737201	1.19665426773468	2.79333201199807
C	-4.94735913139298	-1.17398667185197	-3.20621703151209
C	-4.93561461335805	1.34500451702265	3.14365524173189
C	-1.36408894586486	0.99692439793634	-0.78920193238697
C	0.00996631969154	-0.88341987978734	0.70314442288273
C	0.72064432240166	0.05585706324141	-0.04602778568498
C	0.01967736555352	0.99829002049239	-0.80143443464640
C	-2.12850792926685	-1.94510208581004	1.50958945747181
C	2.19962417911578	0.04797053209339	-0.04470883780909

C	4.16582578368135	0.96804884792852	-0.69627046155690
C	4.15804487064145	-0.88583990944657	0.61036409640435
C	4.90940783953539	2.01327545890545	-1.43038733142906
C	4.89316157206541	-1.93590921354494	1.34626815269954
C	6.30692728583597	1.99965866911115	-1.45698301696715
C	4.22371984529859	3.02762570944385	-2.10486871602884
C	6.29073611299076	-1.93374617139445	1.37232219261060
C	4.19947565956138	-2.94302033585129	2.02334839565342
C	7.00329821766620	2.98155556985157	-2.14569996889669
C	4.92318777907489	4.00882404848137	-2.79147800558060
C	6.97930776120167	-2.91989528336502	2.06282811709752
C	4.89111060512103	-3.92844766352662	2.71186238662801
C	6.31421234465765	3.98861225286046	-2.81420386119875
C	6.28227206519226	-3.91971805951475	2.73389431933907
H	-7.69269280946965	-0.44735248884538	-1.32429120020437
H	-7.68765038414704	0.59574767085804	1.28076191736333
H	-2.88688642729213	-0.92786056194315	-2.61085685783554
H	-2.87785525728102	1.12479426604572	2.53024831132129
H	-4.69502064146282	-1.56413895718933	-4.18387036214054
H	-4.67957130273278	1.74089580887328	4.11803745010230
H	-1.92379053646227	1.72451767166093	-1.36210681949008
H	0.56583634339845	-1.61754655479148	1.26911642995389
H	0.56888216017245	1.72322125411881	-1.38336868936263
H	-2.57312071618239	-1.52178628420590	2.41325859567557
H	-2.94659239156600	-2.36536464273728	0.92273856185400
H	-1.46120918024384	-2.75306149423865	1.80691621090597
H	6.83067553968730	1.21286578896476	-0.93412091943281
H	3.14388427669032	3.03353641248569	-2.07894081795349
H	6.82065860895170	-1.15234281411809	0.84761338926380
H	3.11960619532191	-2.93973965590973	1.99816684912854
H	8.08553984280172	2.96283157378223	-2.16167314439900
H	4.38375847753204	4.79104593041375	-3.31010241820378
H	8.06167226650037	-2.91005111144678	2.07827220073946
H	4.34554463424355	-4.70495047648343	3.23267661499897
H	6.85935338646439	4.75483482374079	-3.35089691142015
H	6.82132280655687	-4.68919720985504	3.27206918721274
H	-7.06412004393698	-1.32431687982641	-3.55033777382632
H	-7.05108478326126	1.47833168196168	3.50225356937325

Table S6. Total energy and atomic coordinates for (4) Cz-TRZ_CH3 molecule.

E=-1568.207480201087

N	-3.52644661280215	0.00054920872475	0.02386634373502
N	2.78210506468892	1.11342181183427	-0.40037485725997
N	2.78650074582472	-1.11907094538658	0.36175124498005
N	4.82579039681502	-0.00372104332258	-0.03381164774488
C	-5.69862725757725	-0.62632480542016	-0.32118392093067
C	-5.69397387970542	0.63259486567445	0.38812579418645
C	-4.34924443311776	-0.98707030173214	-0.52769345731583
C	-4.34194811114894	0.99021852906161	0.58246092355814
C	-2.11958978736665	0.00006931174936	0.01523171253389
C	-6.71592777302901	-1.44567568431973	-0.80897274334976
C	-6.70497852095143	1.45456904786300	0.88448577494068
C	-4.01547710348349	-2.13712130333785	-1.23615550090758
C	-3.99921190268858	2.13988460437880	1.28726002564416
C	-6.40248476419149	-2.60907427082434	-1.50023559888354
C	-6.38269012470406	2.61769323115534	1.57216129507581
C	-5.04993516446930	-2.93056706336964	-1.70864248997818

C	-5.02757739555975	2.93607681260747	1.76837948899783
C	-1.41693216712942	1.13542943467120	-0.39376253184286
C	-1.41270663577287	-1.13588606681022	0.41517868598139
C	-7.48283094844593	-3.52193748427260	-2.01750678262669
C	-7.45624975660312	3.53357294340404	2.09820772274665
C	-0.03338374611854	1.13395529001137	-0.39675281956244
C	-0.02921234553487	-1.13599973168482	0.39940797993077
C	0.68106358522689	-0.00149367216942	-0.00373239261305
C	2.15621649159140	-0.00244595368550	-0.01459211438257
C	4.11703316820016	1.06754540285840	-0.40098892939305
C	4.12135986886081	-1.07448340991926	0.34306715663929
C	4.85444777372237	2.27339687981645	-0.83404919422279
C	4.86386998422663	-2.28142196614095	0.76423468718112
C	6.25170148127433	2.27235967027273	-0.87009695429877
C	4.16284091119368	3.42710125198286	-1.21393633769142
C	6.26146840196432	-2.28071356882108	0.78265832754280
C	4.17690642721852	-3.43597886372281	1.14990770706075
C	6.94236473605811	3.40406096888515	-1.27731871377153
C	4.85646250181532	4.55743369998109	-1.61983951243303
C	6.95702596245056	-3.41348400615954	1.17840137325627
C	4.87541007080619	-4.56745264261188	1.54411853210843
C	6.24735576647365	4.54938386094409	-1.65268777479873
C	6.26660843225186	-4.55968685623981	1.55951360246022
H	-7.75319721212574	-1.17169667637056	-0.65581153077444
H	-7.74419732379051	1.18298475306741	0.74054486225670
H	-2.98594499551575	-2.40406618862684	-1.42765296428845
H	-2.96738921601515	2.40452273923772	1.46944531973557
H	-4.80582120837295	-3.82917953987899	-2.26302055555383
H	-4.77641131967301	3.83445304447401	2.31998340649500
H	-1.96313074236270	2.00701509581664	-0.72631449444860
H	-1.95541370190004	-2.00683943800887	0.75502755592293
H	-7.52358225698876	-4.45258893890836	-1.44438494433085
H	-7.30878069355618	-3.79273422275874	-3.06128450415130
H	-8.46343623673808	-3.04970610336272	-1.95156861668119
H	-7.27162768144846	3.80588493898117	3.13976977989513
H	-8.43836426914552	3.06315767730427	2.04254887241457
H	-7.50069720966997	4.46328641998693	1.52383545521101
H	0.51279551244635	2.00799253086094	-0.71986914993635
H	0.52031883333112	-2.01064647367946	0.71512345718796
H	6.77999873506790	1.37715962784458	-0.57659968066639
H	3.08311843064969	3.42091201990709	-1.18506519822603
H	6.78620059869631	-1.38491271859564	0.48464080931469
H	3.09690482835668	-3.42958376392651	1.13460388706319
H	8.02452369097527	3.39407571255869	-1.30260754538250
H	4.31265043327731	5.44663575281156	-1.91204535995451
H	8.03941768776609	-3.40367311194014	1.19011627221997
H	4.33517156792307	-5.45735004391394	1.84080526209379
H	6.78757215498283	5.43224681929333	-1.97047191256637
H	6.81062025356680	-5.44345809809908	1.86816541259797

Table S7. Total energy and atomic coordinates for (6) Cz-TRZ_tBu molecule.

E= -1804.025037742806			
N	-3.94021278392921	0.00033239064965	-0.03072870908277
N	2.36533307733125	0.84696347900050	0.81566749209924
N	2.37242501362939	-0.89596335282240	-0.77340574179958
N	4.41060168051961	-0.02616703186377	0.03214744521700
C	-4.75150551478929	1.13259867819032	-0.15481480320108

C	-4.76828909083011	-1.12138387284409	0.07653441873712
C	-6.10329697002163	0.73338460902731	-0.12842266978833
C	-6.11401556315457	-0.70479804351275	0.02168536908198
C	-2.53353891594123	-0.00795857714684	-0.01682989122329
C	-4.40814379371394	2.46798333669720	-0.33683397508008
C	-4.44595473374573	-2.46077455804791	0.26743221878842
C	-7.11366188743449	1.68689029448488	-0.25743871010551
C	-7.13897168383880	-1.64495062775203	0.13137813185298
C	-1.83267459371897	0.86751375890534	0.81466669671195
C	-1.82618890323821	-0.89055011311055	-0.83520329833357
C	-5.43490287099180	3.38922921952855	-0.46356966819926
C	-5.48695087393761	-3.36848173102326	0.37499927310465
C	-6.79625315080023	3.03015831505945	-0.42109360218972
C	-6.84241060502350	-2.99183331103728	0.30407909431214
C	0.26583289449402	-0.01977993112519	0.00689101883299
C	-0.44938058664903	0.86394579033997	0.82003947847106
C	-0.44294392716417	-0.89858031086304	-0.81718543975105
C	1.74084083330187	-0.02336457648231	0.01707372359085
C	3.70036030994266	0.81074033811518	0.79390802069452
C	3.70722155288552	-0.86234934662350	-0.73674809121625
C	4.43540882268948	1.75342612897938	1.66409848213378
C	4.45017253176104	-1.80648867923191	-1.59861317367715
C	5.83290547717303	1.75730492427735	1.68032684274581
C	3.74106939239877	2.65099240847379	2.47996269677859
C	5.84776284823313	-1.80872925531990	-1.60381660245868
C	3.76338915502349	-2.70677692097162	-2.41787268548763
C	6.52110283233667	2.64204632131239	2.49688987443311
C	4.43223788586118	3.53447994459700	3.29532572467785
C	6.54346378105858	-2.69423428892271	-2.41316438372439
C	4.46205779845973	-3.59125890322064	-3.22574426248166
C	5.82335841114506	3.53270643081617	3.30627522038864
C	5.85321764845787	-3.58763335785076	-3.22594408339786
H	-3.37640632012320	2.78585407739008	-0.38796845542041
H	-3.41960287687630	-2.79163786479398	0.34039929162917
H	-8.14403866602173	1.36289680235333	-0.23327241969859
H	-8.16432697222183	-1.30767279675943	0.08556495008273
H	-2.38000000979314	1.53408801530163	1.46649696203318
H	-2.36807240511176	-1.55245286900317	-1.49630202545722
H	-5.16621771542843	4.42797231582815	-0.60231080857085
H	-5.23488429648974	-4.41030847617690	0.52164372535019
H	0.09588503963307	1.53592175172919	1.46653576664610
H	0.10751842669426	-1.57488824640281	-1.45471699297194
H	6.36319642688708	1.06079803498101	1.04749912918072
H	2.66107613020389	2.64309206298536	2.46274785239833
H	6.37220557325632	-1.11018378424765	-0.96836980916522
H	2.68327959783418	-2.70020001975161	-2.40924444425822
H	7.60361369384760	2.63797092257802	2.50304594123512
H	3.88623244471377	4.22627316550713	3.92401199167509
H	7.62598352046482	-2.68865468106499	-2.41097200460307
H	3.92187943242234	-4.28523907895193	-3.85705315482221
H	6.36181298546701	4.22306764398856	3.94335238819493
H	6.39751733039013	-4.27863530156423	-3.85733101237046
C	-7.86217026564538	4.12139163135720	-0.56246318483759
C	-7.92535097347679	-4.06833177890747	0.42751213586063
C	-7.79647047383608	-4.77347909054076	1.79122784237688
C	-7.75026661203066	-5.10385965003382	-0.69998844343210
C	-9.33951427180329	-3.48515162719883	0.32361473518991

C	-7.69704683138959	5.14907267215444	0.57363323849248
C	-7.69483318247364	4.83142907662473	-1.91933919616414
C	-9.28573763702456	3.55654744914102	-0.49143942977871
H	-10.00650160604286	4.36976541088415	-0.59379428635041
H	-9.47725515536023	2.84111874433020	-1.29336370900488
H	-9.47695538620893	3.06261919913498	0.46312398857180
H	-7.80899309873415	4.66883699035079	1.54759155402519
H	-6.71643605361507	5.62512312505157	0.54579582357144
H	-8.45308706592114	5.93330023389066	0.48896204575279
H	-7.80967215254226	4.12340120524676	-2.74226604558358
H	-6.71249628311528	5.29550118695311	-2.01239787171827
H	-8.44740751310398	5.61536008177850	-2.03384272660841
H	-9.50333505368562	-2.99237747641163	-0.63662185180272
H	-9.53888629372009	-2.76419242539426	1.11863603961132
H	-10.07304495381818	-4.28841210698466	0.41314990586969
H	-6.82230394366965	-5.24926261761934	1.90813492337914
H	-8.56125298307215	-5.54726712635121	1.89309761009633
H	-7.92041389507875	-4.05982688334963	2.60795499393478
H	-7.83493579618931	-4.62701396612120	-1.67834838589186
H	-6.77727212316376	-5.59342358530587	-0.64900131265904
H	-8.51883823280659	-5.87706592528712	-0.62770569544284

Table S8. Total energy and atomic coordinates for (7) Cz-TRZ_Ph molecule.

E= -1951.621499623019

N	1.75930990860167	-0.00025103525347	-0.00329067401417
N	-4.54818993219453	0.98967788997065	0.65850141835404
N	-4.55216319080210	-0.99827728265594	-0.61198510566016
N	-6.59116819152448	-0.00455411911222	0.03002925519756
C	3.93017478871531	-0.69789267958515	0.16680063910637
C	3.92677694279519	0.70158277584779	-0.19794063545589
C	2.57887286874998	-1.09747207676454	0.27322424587523
C	2.57359899865508	1.09858151205373	-0.28890735190771
C	0.35039250819763	-0.00173158891238	0.00364996304539
C	4.94564541343945	-1.61547618895235	0.41110574149938
C	4.93758600544443	1.62115376983461	-0.45399407086234
C	2.24307432382458	-2.39309306339355	0.65069714536778
C	2.23093179495135	2.39353287237694	-0.66246904922469
C	4.63038169941806	-2.92531431341747	0.77063628820860
C	4.61557453356823	2.93040643705280	-0.80954614654155
C	3.27475358527844	-3.28702500008199	0.89049536152429
C	3.25800814393580	3.28957185672171	-0.91378402561130
C	-0.34999266332084	0.97792436398488	0.70927309734355
C	-0.35465301492367	-0.98260861911827	-0.69559488686489
C	5.69681388676940	-3.91626449604139	1.02971476419298
C	5.67691883901973	3.92366427133852	-1.08034055822384
C	-1.73372815705680	0.97969209485930	0.70671947203206
C	-1.73829743544697	-0.98626701680820	-0.68121690100544
C	-2.44714875310364	-0.00367177906106	0.01563407803683
C	5.55239174721700	-5.25079956078114	0.63491135463091
C	5.53555904723846	5.25690561474150	-0.68016791406651
C	6.88177853377044	-3.54638049936424	1.67555362601011
C	6.85369956526284	3.55734744389839	-1.74293331582871
C	-3.92324497876835	-0.00417789056737	0.02110389399583
C	6.55454543605623	-6.18066177755395	0.87661303720194
C	6.53288001423100	6.18905046906056	-0.93277801272186
C	7.88584314607523	-4.47440257218364	1.91515622247946
C	7.85286283007315	4.48771947098471	-1.99369381889900

C	7.72735049030508	-5.79718400032060	1.51711876431222
C	7.69753565754166	5.80919631628383	-1.59010141039265
C	-5.88366059446864	0.95139573915295	0.63817292249145
C	-5.88747660450859	-0.96034298844664	-0.58276494223288
C	-6.62172592868395	2.03059094653136	1.32746794865162
C	-6.62981112069811	-2.03950581460082	-1.26749787852726
C	-5.93078727021179	3.05793149520517	1.97628925048055
C	-8.01950478589785	2.03574482179827	1.33723291088117
C	-8.02762491184328	-2.04404525227946	-1.26957847027632
C	-5.94287954333998	-3.06727567013979	-1.91988041307068
C	-6.62519104193319	4.07002890039508	2.62179454074351
C	-8.71085544083584	3.04925720805340	1.98378433272252
C	-8.72293760691642	-3.05736225991388	-1.91217220930025
C	-6.64123801554018	-4.07921987326720	-2.56134176427195
C	-8.01648241578460	4.06858924474146	2.62750421190148
C	-8.03253729484998	-4.07713132024709	-2.55947142171554
H	5.98072916366207	-1.31825238427400	0.30308386812371
H	5.97449209092594	1.32606105842369	-0.35818554782977
H	1.21342445087796	-2.69709240333298	0.77370540675605
H	1.19935060145905	2.69549984358501	-0.77367086897478
H	3.02835645121074	-4.29156531273587	1.20772756669215
H	3.00613627884969	4.29373674750097	-1.22790257872234
H	0.19716322992148	1.72248766533547	1.27050855918353
H	0.18866318923052	-1.72630250601388	-1.26169584997841
H	-2.28153551505923	1.73255527394437	1.25412799796287
H	-2.28971569081148	-1.73978143211834	-1.22408345391373
H	4.65586615522415	-5.55616369066692	0.11084703792688
H	4.64556276886769	5.55934667696663	-0.14341771264166
H	7.00529086096730	-2.52617188738142	2.01536953918547
H	6.97431821700172	2.53813391681940	-2.08678783374851
H	6.42246071204361	-7.20625605053623	0.55537653135989
H	6.40349745958265	7.21356957603786	-0.60704478791741
H	8.79046538015268	-4.16549561752277	2.42381702176623
H	8.75107816068054	4.18167300062117	-2.51527671687606
H	8.50930046789155	-6.52165544060330	1.70492341263682
H	8.47569295072304	6.53545945357310	-1.78654285807710
H	-4.85079142529215	3.04803003056622	1.96373866202370
H	-8.54663842232241	1.23878076576676	0.83369240550915
H	-8.55164078482180	-1.24673204811288	-0.76334099262410
H	-4.86282832426115	-3.05780028949497	-1.91327014437077
H	-6.08195080724143	4.86168100496214	3.12169917492142
H	-9.79332280807121	3.04562437124379	1.98644304848413
H	-9.80540196678480	-3.05322699923113	-1.90897549234928
H	-6.10108361218939	-4.87122031666316	-3.06402760019397
H	-8.55777020616197	4.85912809391768	3.13175862398132
H	-8.57693084273701	-4.86750787664027	-3.06062992790661

Table S9. Total energy and atomic coordinates for **(8)** Cz-TRZ_CBZ molecule.

E= -2005.779215887983			
N	-6.02943198790973	0.58978372300410	-0.47968643602038
N	-1.08024394291424	-1.56136798980690	0.85682855814152
N	5.13965564718607	-0.77261309806510	-0.52069019967821
N	4.64729812790830	1.31124474819355	0.46879261296468
N	6.82760363677049	0.85909655468637	-0.30539680225021
C	-3.36477360430325	-1.59445880785589	0.85324621322142
C	-2.21989216556107	-0.86259445876068	0.45898437835350
C	-4.74643898637205	0.08450018545563	-0.14979395594778

C	-2.89356698167827	-2.78423737264358	1.52400209040010
C	-1.48035452372255	-2.73266257221214	1.50542228080849
C	-6.97860762526571	-0.05844747142537	-1.26561756084342
C	-6.54803970915755	1.81641066122286	-0.07519868726739
C	-4.63319385309852	-1.10502250521579	0.55701682032245
C	-8.12621861669134	0.76409979042268	-1.37014659538857
C	-7.85130847661010	1.96182064986290	-0.60913299383812
C	-2.33042320078390	0.32796426794584	-0.25246909133902
C	-3.60301206966583	0.78639918096539	-0.55686445975516
C	0.25381534410515	-1.14878306550308	0.65301211713424
C	-3.53627370791886	-3.85638907563818	2.14039336139445
C	-0.70815015932293	-3.72105054961322	2.10724890624077
C	-6.90156928362002	-1.29083033886273	-1.90647013305979
C	-5.97763771015536	2.79135845929034	0.73679174350585
C	-9.21373956860257	0.32921178474841	-2.12591343106071
C	-8.58190822678202	3.11464465551362	-0.32671955750966
C	-2.77100938133800	-4.85150910754873	2.72848378011666
C	-1.37273476730001	-4.77791081896093	2.71413461960465
C	0.66424384747439	0.12221946488239	1.05511853931412
C	1.17024644801178	-2.01264861121947	0.05367080424360
C	-7.99873140494708	-1.69897055084327	-2.65255165793734
C	-6.72779431471786	3.92895543423858	1.00217685608758
C	-9.14532606254353	-0.90190854933692	-2.76129523654498
C	-8.01503303169343	4.09400281179169	0.47552246204506
C	1.97401578982089	0.52315039170432	0.85608133534054
C	2.48179379616476	-1.61152536871150	-0.13252642412585
C	2.90100729280083	-0.33890677745795	0.26409616741645
C	4.30041410570670	0.08806801939259	0.06074800560126
C	6.39462480554204	-0.34482241090941	-0.68936468829428
C	5.92294546671972	1.65627742054783	0.26929187812361
C	7.35924333274755	-1.25586766606711	-1.34049341538245
C	6.35799349095712	2.99858745033480	0.70862988177199
C	8.68129211728979	-0.85303696927545	-1.54970707709600
C	6.95961502289534	-2.52849453652889	-1.75800575803175
C	7.68643672156730	3.40031606027011	0.54212927186605
C	5.44629547776005	3.88191761953530	1.29357194347376
C	9.58468567858588	-1.70778751518769	-2.16319151844426
C	7.86549745628221	-3.38086288502769	-2.37120591831745
C	8.09351807792886	4.66035763465482	0.95393839248841
C	5.85629691208916	5.14181877543003	1.70300961681009
C	9.17999265503370	-2.97344078831138	-2.57517600326881
C	7.18029005790731	5.53459419493751	1.53472209887425
H	-5.52512702595076	-1.63555753292758	0.86267486457383
H	-1.45656815278755	0.87250802175872	-0.58057439573644
H	-3.72750074388181	1.69765885040726	-1.12595696224302
H	-4.61753636888048	-3.90815899419173	2.16355848427630
H	0.37126209366883	-3.66793158248798	2.11292529520687
H	-6.01615908828101	-1.90669069894565	-1.83008479891419
H	-4.98697978511176	2.66492771258379	1.15151989414796
H	-10.09925119958561	0.94582416406062	-2.21769829536016
H	-9.58033918119715	3.24276127804087	-0.72617985192844
H	-3.25577085941227	-5.69075171789752	3.20942505225506
H	-0.79432609613337	-5.55995762636450	3.18896365806899
H	-0.04384604935465	0.78191466180474	1.53751886513079
H	0.84363219489167	-2.98974331623199	-0.27465482429543
H	-7.96475590613211	-2.65379723091880	-3.16160230682357
H	-6.30806092754873	4.70313084415391	1.63185235343894

H	-9.98315249347563	-1.25163268253447	-3.35024387405014
H	-8.57190539687669	4.99389352675189	0.70176611660515
H	2.30051750798751	1.50324316609825	1.17147360403397
H	3.19576929079816	-2.27386363132479	-0.59953517883379
H	8.98349754303223	0.13252324258346	-1.22718194291261
H	5.93648540440961	-2.83400960909341	-1.59484347436735
H	8.38627468407148	2.71316515429480	0.08963148464959
H	4.42102907884826	3.56609969934014	1.41939350928475
H	10.60639656827606	-1.38714120897673	-2.32175411529226
H	7.54708320445433	-4.36452556202969	-2.69187014329358
H	9.12441268967125	4.96286270441528	0.82132891646854
H	5.14298937566953	5.81968022638081	2.15409477085367
H	9.88643302387636	-3.63965150403611	-3.05407364291932
H	7.49918866837466	6.51836956724389	1.85527980371192

Table S10. Total energy and atomic coordinates for (9) Cz-TRZ_DPF molecule.

E=-2951.889487698579

C	8.55278865167573	4.24750424162800	-0.15072276395273
C	8.46921420766453	2.77576179222876	-0.21506963503631
C	7.77668190548075	2.14743732202098	-1.25406618120227
C	7.69860340891922	0.76748853395038	-1.31846937794654
C	8.30429672935444	-0.01560668203633	-0.33434045742563
N	8.21741452195706	-1.41949466019125	-0.39118488148862
C	9.28613054489790	-2.31149061206162	-0.25890882048941
C	10.64977675984351	-2.06761227684612	-0.12712924232766
C	11.50107827736046	-3.15990976604012	-0.06728389338357
C	11.03387730618203	-4.48462669801030	-0.13930047248834
C	12.02236648905598	-5.64553119702287	0.02278229485549
C	12.26963741904005	-5.86992373152416	1.52000563172795
C	12.80425026552427	-4.99743222601896	2.45087420129019
C	12.92066491899844	-5.40995374928281	3.77704048096769
C	12.49967504606898	-6.68086083023614	4.16441779675547
C	11.95812272882020	-7.55948721085683	3.23238828323152
C	11.84584391689135	-7.14857727546666	1.90827088884664
C	11.32765471619366	-7.84973235912927	0.73215512199806
C	10.80670587233733	-9.13227651814882	0.59537568423622
C	10.38263857581940	-9.55458412876358	-0.65986909858754
C	10.48483491902069	-8.70933164723864	-1.76341528364036
C	11.01112936645180	-7.42611832174778	-1.62681498794917
C	11.42269718994629	-6.99901785431319	-0.37724581658974
C	9.67154678603259	-4.71000188785052	-0.28139543215328
C	8.79371088748344	-3.63063049467291	-0.34792822520900
C	7.36487469173775	-3.53522585652377	-0.53510898010375
C	6.35959632442857	-4.49054076759767	-0.66421335644792
C	5.04057993341756	-4.08755658666874	-0.82186909674051
C	3.89658869390743	-5.10640942932526	-0.88401265886972
C	3.31640140891117	-5.27800981768185	0.52557779602526
C	2.72191726747959	-4.33089890926307	1.34000057862814
C	2.27508024942703	-4.70975772432007	2.60459011367754
C	2.42826386746205	-6.02236348124411	3.04760827653866
C	3.02951971256360	-6.97628925343837	2.23371043128262
C	3.47224038909981	-6.59830622097285	0.97040658769006
C	4.12767597764956	-7.37536086314597	-0.08306909225157
C	4.49102547221133	-8.71729617687572	-0.12885006774313
C	5.11128029045533	-9.20638634287833	-1.27328421076927
C	5.35891897739442	-8.36733364818608	-2.35836638260483
C	4.99047631028366	-7.02411231985200	-2.31375522597791

C	4.38284568968670	-6.53200198115742	-1.17269930375931
C	4.74521820322349	-2.71287742913085	-0.83099187481197
C	5.72483967055097	-1.74089154210781	-0.69950999130442
C	7.04401297710025	-2.16124145325676	-0.56199683293737
C	8.99539639577226	0.60442491730656	0.70831824095033
C	9.07979631038882	1.98445814974326	0.76201290441359
N	7.94770120402406	4.95234082868717	-1.11091883142333
C	8.04992652676063	6.28094775090159	-1.01674035455269
C	7.40064919501229	7.10394148810146	-2.05883803390511
C	7.48029686470941	8.49853107994534	-2.00966960671403
C	6.87164359082861	9.26907718234767	-2.98906781153662
C	6.17677745078952	8.65767487661051	-4.02791228932615
C	6.09277800982875	7.26997305949243	-4.08274019864111
C	6.70047704471826	6.49662244236587	-3.10502962431026
N	8.70411556389428	6.90967261313953	-0.03633157593207
C	9.27673354652755	6.12951810823086	0.88461037868461
C	10.00669920176174	6.78261586161414	1.99177328997664
C	10.62471756558431	6.01452380356772	2.98261705075420
C	11.30733101702005	6.62969303109872	4.02146097015326
C	11.38169111854201	8.01765490377606	4.08347773080172
C	10.76927175673773	8.78850992058986	3.10048314975749
C	10.08570250995234	8.17643616048482	2.06046588452582
N	9.22774075722542	4.79465269975917	0.86432595459223
H	11.04445911979301	-1.06234889883287	-0.08760010246296
H	12.56418568102957	-2.98159999925669	0.01778599966824
H	13.13062578685033	-4.00770510715480	2.16041338447320
H	13.33955305362046	-4.73603020785364	4.51333264686670
H	12.59433289975724	-6.98484896256952	5.19910383492858
H	11.63010321405273	-8.54584499370739	3.53583736053817
H	10.73009536626130	-9.79323733181626	1.44972406476727
H	9.97301001983673	-10.54903393479072	-0.78285134951807
H	10.15457329866831	-9.05298450662350	-2.73523057511552
H	11.09137279214390	-6.77566614273825	-2.48801893572539
H	9.28814377581111	-5.71820800360813	-0.34815034453338
H	6.61093843647797	-5.54139817969961	-0.63557645970355
H	3.71888326862243	-2.39713233908723	-0.95848359703912
H	2.60057954878480	-3.30907678849267	1.00594971405993
H	1.80696166420423	-3.97694266177405	3.24924170456260
H	2.07808935358775	-6.29966593636250	4.03372124681164
H	3.15021667490076	-7.99491302987035	2.58081056898215
H	4.29704477383267	-9.37262986712003	0.71112455903867
H	5.40216114034452	-10.24787610997606	-1.32395210055025
H	5.84017193048843	-8.76253297768265	-3.24373224772408
H	5.18240849431344	-6.37878636970268	-3.16083423612061
H	5.45923965127565	-0.69343918767703	-0.70033484145366
H	9.44595293877315	-0.00207463774300	1.48160926028900
H	9.60659112146342	2.46873872769570	1.57107844756411
H	6.93858903489692	10.34852673336548	-2.94336869902107
H	5.55263337700550	6.79097061233820	-4.88930275455731
H	6.64243157752465	5.41855077439515	-3.13660067074255
H	11.78262751277392	6.02681720359381	4.78463806801576
H	11.91479292696662	8.49679548746699	4.89492011693620
H	10.82506238570842	9.86860868220220	3.14578145736247
H	9.60571837156437	8.76411853598576	1.29181728519799
H	10.56008073025653	4.93791690033507	2.92404774167543
H	8.02274960778202	8.96131867366072	-1.19834308511590
H	5.70216439546244	9.26053780197468	-4.79181589562244

H	7.31363707811422	2.75713314202365	-2.01597483550166
H	7.18437560785504	0.28671290211477	-2.13890926094950
C	2.84327648815777	-4.73257828911497	-1.93229801788757
C	3.23933347528827	-4.21851719208857	-3.16862135633663
C	1.48758427698240	-4.97399514781622	-1.71885833976555
C	2.30696622198863	-3.95055590765083	-4.16163174144699
C	0.55112929254845	-4.70280589370149	-2.71065732942300
C	0.95580721269290	-4.19023965369894	-3.93637218321736
H	4.28581113172256	-4.01299729780324	-3.34995761222984
H	1.15862783696430	-5.37752561909024	-0.77140870731149
H	2.63691303630134	-3.55009171757666	-5.11211053582409
H	-0.49774457422417	-4.89356028975353	-2.52109409665793
H	0.22691228411518	-3.97672199479593	-4.70770027095763
C	13.31020137398188	-5.43383943640988	-0.78007262351230
C	14.53973946816435	-5.88808009102571	-0.30628655542532
C	13.25909455974595	-4.86203646873842	-2.05254845777764
C	15.68926365256191	-5.76799334291711	-1.07916441922626
C	14.40542642030465	-4.74257102717645	-2.82705178448860
C	15.62801257725130	-5.19390322829116	-2.34261776726999
H	14.60123907082513	-6.34014613934751	0.67395927883950
H	12.31615963439792	-4.49461859749401	-2.43466693391569
H	16.63456723914411	-6.12430451019401	-0.68941500190722
H	14.34304138270951	-4.29282808195908	-3.81012934533406
H	16.52328291748103	-5.09641927587348	-2.94329540603356

Table S11. Total energy and atomic coordinates for **(10)** DIPz-TRZ molecule.

E=-1773.572055276209

N	-2.70509283639561	1.18036196176078	0.47115181836266
C	-4.09222097932487	1.27549494054937	0.60310411848755
C	-4.93771691358323	0.97935255750885	1.68064254865850
C	-6.30928898421447	1.17837997856142	1.51500754831978
C	-6.84504591399596	1.66171152124941	0.30820875500704
C	-6.00652084256577	1.95682761839431	-0.76512372256806
C	-4.62724308141341	1.76609753419684	-0.62567004603983
C	-3.51585314995693	1.97281513040292	-1.53177974616010
C	-3.38167286109959	2.42617490309284	-2.85637879462734
C	-2.10446638346353	2.48640297673044	-3.40364679543757
C	-0.95626205152635	2.10977699851634	-2.67234754378805
C	-1.07140650208174	1.65880968221592	-1.35628994447751
N	-0.03899891237296	1.24755221539637	-0.49343626487093
C	1.34131299422232	1.15407313325828	-0.62595781177599
C	2.19174223096232	1.45522724494798	-1.70140470361214
C	3.55780742703423	1.25668182769974	-1.53708069180855
C	4.10371819690301	0.76460421218965	-0.32987617047421
C	3.25183882672254	0.46622533772566	0.74191894040236
C	1.87961154560108	0.65830378779285	0.60185049749378
C	0.76864009054065	0.44865359303606	1.50927835774695
C	-0.37838635316138	0.82166587716694	0.79660558554041
C	-1.67576917695963	0.76600472615404	1.33278085247526
C	-1.79007232675540	0.31010912189705	2.64786145390486
C	-0.64201299294692	-0.06939497342399	3.37790702447097
C	0.63596293281978	-0.00856107018082	2.83233340509846
C	-2.36774573208512	1.60228880729254	-0.81700932292915
H	-4.55995959419169	0.60377875392892	2.62946964252047
H	-6.97972777931125	0.95064647178445	2.34913861417432
H	-6.41622745539676	2.33308439874752	-1.70697398259875
H	-4.25684414231523	2.72218296426857	-3.44018961430920

H	0.01633362951080	2.17629598944885	-3.15349293711537
H	1.81727381393164	1.83645959379701	-2.64905483358741
H	4.24238513634576	1.48263565351965	-2.35615883196400
H	3.67803741262246	0.08725942805060	1.67215820519796
H	-2.76265631620993	0.24148456313234	3.12869523816001
H	1.51169649097124	-0.30615388506154	3.41420085884673
C	5.56104424918051	0.56600665228641	-0.19845714633406
N	6.03081601125350	0.08778616012056	0.96187562598364
N	6.34011022340996	0.87222672379924	-1.24425120069591
C	7.35474711098136	-0.07980153190280	1.04016582475592
C	7.65300295835697	0.67603236032316	-1.08154666503255
N	8.20218635805266	0.20168873118530	0.04287799620906
C	7.91840970970419	-0.60924214358482	2.30540371364707
C	7.07360089278985	-0.92166580087536	3.38357085177269
C	9.30325621368938	-0.80455974007174	2.43859642691484
C	7.60488627725195	-1.42054874693779	4.57284852351989
C	9.83260610863595	-1.30358618275346	3.62880155667839
C	8.98534819551748	-1.61288232377424	4.69872648431244
H	5.99930661956737	-0.76628069050816	3.26982404699484
H	9.95066941675117	-0.55871068069550	1.59507920785820
H	6.93981095532697	-1.66160046951795	5.40777069739347
H	10.91249837125735	-1.45281834806268	3.72410782976121
H	9.40154113265454	-2.00454423083377	5.63228790480529
C	8.55357824257570	1.00406685554132	-2.21297717206643
C	9.94037410757974	0.81263293356135	-2.09472705740187
C	8.02969776749934	1.51013013635261	-3.41433307888390
C	10.78702506363858	1.12198265633276	-3.15927138342782
C	8.87809587581051	1.81908705510298	-4.47755222745472
C	10.25854495363617	1.62593336779626	-4.35301169046350
H	10.33710145197508	0.41903225685284	-1.15726629495738
H	6.95105769264386	1.65526959610228	-3.49578823537879
H	11.86605734797377	0.96981947151612	-3.05895780742878
H	8.46189055774676	2.21312731685215	-5.40978769543091
H	10.92364843698299	1.86868611267766	-5.18777426643748
H	-0.77581645115573	-0.42078559261576	4.40496059815734
H	-1.97147405731047	2.83458451087680	-4.43184165339782
H	-7.92505499483763	1.80560167710610	0.21429904730371

Table S12. Total energy and atomic coordinates for **(11)** CH₃_Cz-TRZ molecule.

E= -1723.027847681384

N	-0.19115173046398	-1.12229869098666	0.18310031217095
C	-1.25468562869151	-1.88348420600922	-0.21607755203286
C	-2.40698559952048	-1.34594685062320	-0.76921596267523
C	-3.37734535173937	-2.29495187183868	-1.11018243501555
C	-3.15670436863012	-3.67308136053594	-0.89234218063763
C	-1.97148877628353	-4.16651444467273	-0.33217070223331
C	-0.97210041594084	-3.25049134283712	0.02466926808394
C	-2.50566935440415	0.17929456225382	-0.95129754838612
C	-1.22658241053816	0.91908155480039	-0.46458017521908
C	-0.11678958665101	0.24074879100480	0.08514787271609
C	1.06481609024412	0.86598288913347	0.53983185092901
C	1.10972623098690	2.25250178653227	0.42549661817715
C	0.03429147427153	2.97983354660909	-0.11443061994703
C	-1.11874369058658	2.30410537221407	-0.55153733018907
C	2.25624431697106	0.06992177588657	1.14566541225415
C	2.00274025011822	-1.44855242559875	1.15665292613394
C	0.79408227072651	-1.93114304199128	0.67807164365537

C	0.37259889368222	-3.28183959821425	0.61058042452718
C	1.27812149755418	-4.24234267892279	1.08246543088453
C	2.51368022829680	-3.80540126976799	1.57687117901379
C	2.87609165478133	-2.44067356211485	1.61645167509172
H	-4.32634465702097	-1.97960175763633	-1.55387747679483
H	-1.83793192890031	-5.24135551720149	-0.18121980875713
H	1.98385290770742	2.81567520850882	0.75407585064906
H	-1.92909664160968	2.90632627522418	-0.96363026605564
H	1.03494960440596	-5.30843489664891	1.06825293516752
H	3.85799108678090	-2.17025619217572	2.01607265691138
H	-3.94392271215166	-4.37844249318322	-1.17462353895257
H	3.22862844338035	-4.54593584532019	1.94752940755478
C	3.52449074755457	0.35492885277845	0.30898647078597
H	4.39340660514566	-0.18506525306866	0.72447892407946
H	3.38428715932908	0.02776768320559	-0.73536748897565
H	3.76562906392424	1.43198632320467	0.30387378915801
C	-3.71731466530041	0.69738512238461	-0.14220952629507
H	-4.64683189372014	0.20306032832125	-0.47529636871451
H	-3.58492769291510	0.49083908221468	0.93354101327691
H	-3.84439923177841	1.78627288309174	-0.27119570810075
C	-2.71520585879639	0.48363867563492	-2.45330333643141
H	-1.85590607710722	0.12737646690513	-3.04660246420155
H	-3.62379234092433	-0.01962346999440	-2.82792487969697
H	-2.82958887159472	1.56753212913983	-2.62772657537136
C	2.47544803273698	0.54111543984658	2.60233566728720
H	1.57907626171503	0.34247772614401	3.21418474022271
H	3.32814395265798	0.00807076475538	3.05879794948153
H	2.68734900868237	1.62383294030257	2.64270874453590
C	0.11642700535653	4.44828128037071	-0.22390605740744
N	1.23314924889977	5.05479365745951	0.20280552815028
N	-0.92928790435825	5.10483316717894	-0.74594922727253
C	1.26742697727492	6.38552762368438	0.08257383684655
C	-0.81271839411345	6.43368385742875	-0.82919178409742
N	0.26751506194995	7.11480899899283	-0.42764528367169
C	2.48590749844290	7.09628412215650	0.54031303823145
C	3.56454508775378	6.37924058479144	1.08460271482248
C	2.57440302007177	8.49425237182572	0.43356425581142
C	4.71026194653154	7.04894662377129	1.51412777437556
C	3.72114412844372	9.16215196719442	0.86359325313188
C	4.79173721204378	8.44176553415797	1.40488242434919
H	3.48658780491759	5.29345242579590	1.16312847631020
H	1.73121440617554	9.04208827825494	0.00927847013476
H	5.54588040712522	6.48281595318213	1.93698429839955
H	3.78171671212504	10.25128781386295	0.77666475756949
H	5.69119987970577	8.96655350578361	1.74208247579583
C	-1.94682025600026	7.19919461938842	-1.40119835689771
C	-1.87486048149288	8.59778399937730	-1.51230379356045
C	-3.10449939043361	6.53390696375788	-1.83819979190426
C	-2.94184199269536	9.31707658238196	-2.05098053162759
C	-4.17035602054128	7.25494403379879	-2.37644004566564
C	-4.09198111342539	8.64804679775282	-2.48429535666648
H	-0.97119563679796	9.10503369260955	-1.16992291131500
H	-3.15086145121100	5.44725453532980	-1.74781620523282
H	-2.87751806857752	10.40630519842865	-2.13408690038367
H	-5.06850887964140	6.72893432532822	-2.71436607756336
H	-4.92875808291382	9.21319370819986	-2.90684242872748

Table S13. Total energy and atomic coordinates for (12) Cz-TRZ_7 molecule.

E= -1644.409257584770

N	-2.18695554337176	-0.31072028389268	-2.80142351874178
N	3.02661610224093	2.60664451018476	-0.26462236092514
N	3.98424699636210	1.59612443953125	-2.17300414923822
N	5.33066128355195	2.86626293277987	-0.70797433232026
C	-3.45371196065086	0.30448778938221	-2.60526896195952
C	-2.42341568148251	-1.57854718247436	-3.40138541394948
C	-4.46292190736355	-0.55684894795293	-3.09930954734011
C	-3.81992015327994	-1.76170945750970	-3.54845126713924
C	-0.91645598494832	0.23391703977322	-2.44927913109557
C	-3.81684639439041	1.53086580600670	-2.00795937714323
C	-1.53899312751563	-2.57716874218652	-3.86303779642340
C	-5.81282234755331	-0.18973269678635	-3.10050037735462
C	-4.36131452244504	-2.94940391006555	-4.05122686739940
C	-0.75932776211696	1.02818833437010	-1.28192296091164
C	0.22669605345241	-0.00456197914901	-3.25744700914676
C	-5.17375746825002	1.87490732123728	-2.03081272332434
C	-2.10998907568623	-3.75803986842272	-4.35335356044855
C	-6.16476048438464	1.05122636472953	-2.58475378002296
C	-3.49460871048766	-3.96677962262488	-4.43056168048250
C	1.62437340256108	1.30926226274796	-1.74347014219656
C	0.49413800385169	1.54937187238325	-0.95970214271861
C	1.46309493504374	0.52608225525638	-2.88778526556876
C	2.94225806171850	1.86445630105286	-1.37593655116397
C	4.23868774126238	3.08753724351968	0.03362494187075
C	5.15968669290909	2.11684948196271	-1.80362273059150
C	4.38089787124574	3.91306158598194	1.25670568128280
C	6.34177857222768	1.84783457264587	-2.65680413156994
C	5.63261674051277	4.44045926299289	1.61571673939396
C	3.26527770058968	4.17623926647244	2.06919767320817
C	7.60063407975123	2.36604042987955	-2.30953881028180
C	6.21494445179600	1.07231582637890	-3.82146649750405
C	5.76514567625685	5.21701601931655	2.76685988211742
C	3.40001261245311	4.95318691714888	3.21975788931788
C	8.71215869138566	2.11237109364746	-3.11320712753010
C	7.32766761931455	0.82022292097262	-4.62388901682491
C	4.64980933246675	5.47541033812531	3.57162771230026
C	8.57881882742641	1.33920077629179	-4.27201653616097
H	-6.56756110519721	-0.87200122541686	-3.50124193150807
H	-5.44507177770175	-3.06537918189142	-4.13972528574285
H	-5.46774610406830	2.81980110920799	-1.56259692192654
H	-1.43345446596151	-4.53604446932544	-4.72149844505338
H	-7.20949849816752	1.37483370036116	-2.57596644019749
H	-3.88211371199641	-4.91217275443666	-4.82093806362725
H	0.60268123673376	2.16248495151014	-0.06350022910079
H	2.33618923541462	0.33064613853480	-3.51255024694345
H	6.49276738164406	4.23014995037117	0.97775907843965
H	2.29764819896798	3.76132507318725	1.78154238716931
H	7.68815669614234	2.96718119735297	-1.40283082494766
H	5.23251445902637	0.67474833171019	-4.08216861620631
H	6.74361119455217	5.62414674886051	3.03946483013878
H	2.52614198210987	5.15342194256412	3.84722221322845
H	9.68919022401673	2.51962676894114	-2.83569289683364
H	7.22033261205006	0.21564096348727	-5.52967335030246
H	4.75480302746374	6.08481196654311	4.47479179531766
H	9.45154828586902	1.14088273204156	-4.90215995348774

C	-1.91156498981234	1.44823915201344	-0.41113385689323
C	0.20980529329801	-0.90819893939940	-4.45949033848058
C	-0.05907156248912	-2.35905794804402	-4.02108020117011
C	-2.85940606860460	2.36703695833547	-1.20452590033074
H	-2.25650238510849	3.04437326795651	-1.83734093032849
H	-2.48044931397701	0.57996620346626	-0.03324926622463
H	-0.55723452074319	-0.60219643065482	-5.19327519470409
H	0.32128179868447	-3.06681285146711	-4.77686114597624
H	-3.43932613895226	3.00831353987042	-0.51958129011495
H	-1.51139744830717	1.98135268949618	0.46525167272987
H	0.49964368741746	-2.56179675178318	-3.08857846109147
H	1.18675319224270	-0.83875062810003	-4.96272255784485

Table S14. Total energy and atomic coordinates for **(13)** ICz-TRZ molecule.

E=-1488.378034138231

N	4.09812069397479	-2.86427716662666	0.07307752063992
C	4.97054013431489	-2.71976926723419	-1.01576636563762
C	5.68908535365027	-1.61123809457511	-1.45470278984573
C	5.04058209783111	-3.98827396613411	-1.69546313211978
C	3.65756458729365	-4.15041211289868	0.06042565763542
C	4.16774207582672	-4.92398617129890	-0.97325317313167
C	6.49295098585306	-1.76302999750164	-2.59040811242698
C	5.85302911953016	-4.10334290584684	-2.82525615335406
C	2.77231336136702	-4.46603035125165	1.08210574170997
C	6.57525832586015	-2.98985481764035	-3.26718069009752
C	3.70731635921335	-6.24359982316860	-0.97758504123988
C	2.32408823598470	-5.78963665451447	1.05890718766577
C	2.79585072872676	-6.65649023493822	0.03403726318308
H	7.06744959275382	-0.90627983407040	-2.95515473995911
H	5.92176856983740	-5.05646043040781	-3.35727505848586
H	7.21281072012561	-3.07520420327598	-4.15186637785351
H	4.01259348780754	-6.97839971996255	-1.72312456499554
H	1.62570157988276	-6.19395908647529	1.79228486963778
C	2.03768693103551	-1.50134931402204	3.42072054130247
C	2.85938869954096	-0.57103227545133	2.76551396450640
C	1.92979474823681	-2.81631129850223	2.95600187333161
C	3.59656001199988	-0.92465556680707	1.62949205919379
C	2.65104858109279	-3.20423183743365	1.82505461830989
C	3.48869832656754	-2.23350838573793	1.16778019883750
H	1.28727475068689	-3.53611851312599	3.47111710770721
H	4.23457714929392	-0.19683885187547	1.12327960594343
H	5.62841416625391	-0.65430693608592	-0.93169880673386
H	1.47463601639691	-1.19281522046523	4.30626209659506
H	2.92726629815210	0.45185360984422	3.14783737136224
C	2.31384645990248	-8.05731986718469	0.01855937462497
N	2.76662593978881	-8.87441517051548	-0.94215329978491
N	1.44743982736910	-8.44163359875944	0.96574912039755
C	2.30663270035349	-10.12950987184239	-0.92063440430729
C	1.03684505467955	-9.71297382989813	0.91530767957712
N	1.44085392084909	-10.59087624552870	-0.01042839550067
C	0.07732363810114	-10.17850657466652	1.94573553784349
C	-0.38457756843470	-11.50526306622688	1.93713763882765
C	-0.37970295331514	-9.29836756843179	2.94080800674099
C	-1.28724401604939	-11.94288882416614	2.90642685220522
C	-1.28237031545822	-9.73786374115858	3.90914669127048
C	-1.73849586657937	-11.06080291486542	3.89465341085594
H	-0.02326297284447	-12.18092965403329	1.15993873330600

H	-0.01488853446962	-8.26979200552209	2.93891746798271
H	-1.64198219925443	-12.97799349919135	2.89244933097965
H	-1.63331497074244	-9.04568470293513	4.68064516482640
H	-2.44679431893156	-11.40489470801115	4.65492670276942
C	2.78348200608613	-11.06639519563543	-1.96662991341835
C	3.69909893872300	-10.63720139114448	-2.94192668929172
C	2.32405884226803	-12.39379725679202	-1.99260053249595
C	4.14658688154769	-11.52010832278058	-3.92473864931893
C	2.77249610168619	-13.27511990121865	-2.97645376523012
C	3.68467043097321	-12.84096216186489	-3.94479890602108
H	4.05036675522988	-9.60430427068003	-2.91334001873200
H	1.61289660272028	-12.71704579520045	-1.23046806800846
H	4.85991819545645	-11.17772450463578	-4.68067476551649
H	2.40932355154194	-14.30730754220956	-2.98944149926177
H	4.03612905271174	-13.53314476041648	-4.71645360700027

Table S15. Total energy and atomic coordinates for **(14)** QA-2CH₃-TRZ molecule.
E=-1724.218010147423

N	-0.20363685404528	-1.21967736857092	0.11801684298658
C	-0.88305978427562	-1.88024356946211	-0.92704266660280
C	-1.91202250875644	-1.18972138036679	-1.59916711654900
C	-2.50835622937785	-1.80570799006760	-2.70511997467588
C	-2.12440806443779	-3.08264179139678	-3.12352827965190
C	-1.11247091717937	-3.76004057430594	-2.43852765856295
C	-0.48320043248749	-3.15641701185720	-1.35107392798524
C	-2.35205632208489	0.16004220616367	-1.03029022520020
C	-1.09615636303744	0.91375666529166	-0.58967460926003
C	-0.08077895185652	0.17286290082381	0.04565400974366
C	1.05352791869825	0.78782203124223	0.60985949714985
C	1.14804853436486	2.17439595696208	0.54334990162380
C	0.16603990294256	2.93775247541215	-0.10753369570176
C	-0.94355295283254	2.29391277617671	-0.67781847676132
C	2.16000558559987	-0.12099105913508	1.14733645770642
C	1.49505305098234	-1.31050113647328	1.84231328229586
C	0.35898779825400	-1.87858143801726	1.23115011358678
C	-0.25097941214002	-3.01844957065983	1.77653160476766
C	0.27154586634979	-3.60786310573633	2.92646404588130
C	1.38839641583303	-3.04801512974800	3.55202746703561
C	1.98316828615716	-1.90485576907477	3.01152565944846
H	-3.30072015359722	-1.28955331926062	-3.24986354799689
H	-0.79496033782117	-4.75591040018709	-2.76221378845203
H	2.00083967443208	2.70182653149484	0.96692242891424
H	-1.69439951183391	2.91353408518402	-1.16487704856451
H	-0.21048108020613	-4.49677452669853	3.34453404458027
H	2.85548314920713	-1.47941306273101	3.51030756780056
H	-2.61545713638722	-3.54482492108127	-3.98475188414589
H	1.79759654549128	-3.49809550930310	4.46111051915810
C	0.29994237077577	4.40409451066166	-0.19162073426072
N	1.36588644043426	4.97757077526864	0.38470914335946
N	-0.64999781832764	5.09250016616934	-0.84040061617849
C	1.44959390403240	6.30759223981163	0.28504277483337
C	-0.48950699846349	6.41835400348184	-0.89265604507757
N	0.54462351834171	7.06752570485882	-0.34382113481920
C	2.61424343261213	6.98168423777793	0.90873559286646
C	3.59068086176093	6.23120839812653	1.58496709840564
C	2.75304891216642	8.37735064325288	0.82990609088580
C	4.68563806822846	6.86598533817749	2.17130201555783

C	3.84894507450213	9.01027573562901	1.41682096422369
C	4.81785829120776	8.25676828579439	2.08883333895082
H	3.47306546729972	5.14755831246310	1.64115621731156
H	1.98884300915155	8.95075828034328	0.30229695594292
H	5.44153543989393	6.27409788227083	2.69658983054137
H	3.94938877073700	10.09795729730212	1.35066047137376
H	5.67734408486426	8.75418923578260	2.54931671211620
C	-1.51762120053968	7.21808877037916	-1.60197356993291
C	-1.40384907109956	8.61636634774571	-1.67479612714264
C	-2.61535116537937	6.58545911346464	-2.20914257615873
C	-2.37122120033280	9.36766636489481	-2.34245150562235
C	-3.58124764433484	7.33843246904759	-2.87677338664198
C	-3.46202407814663	8.73114746687840	-2.94512279656347
H	-0.54712126001240	9.09773331905798	-1.19991941233977
H	-2.69368424170391	5.49858512399793	-2.14764532325868
H	-2.27519185508042	10.45653167825446	-2.39414850058860
H	-4.43275052141774	6.83760461763317	-3.34766045914679
H	-4.22046063872325	9.32131933802419	-3.46921127080851
H	0.33281926052069	-3.66440893117221	-0.83320379641379
H	-1.14460135141021	-3.42967350158640	1.30277350529974
C	-3.21038532412359	-0.11161135008180	0.23634604472297
H	-4.11589967733504	-0.68460965701083	-0.03226535992928
H	-2.64574751005690	-0.69125812838029	0.98539214524808
H	-3.51668849097053	0.84272515473283	0.70041295176908
C	2.96166501467152	-0.66361010809001	-0.06827107864165
H	3.74868082737657	-1.35901683158238	0.27432036448464
H	2.30612247241016	-1.20455269270512	-0.77097026558231
H	3.43536066321425	0.17114797318947	-0.61480111338987
C	-3.19316506907063	0.97161206579568	-2.02292212895461
H	-2.62925600529069	1.20350877581798	-2.94267365845408
H	-4.10795588272127	0.42333563467239	-2.30167957523098
H	-3.51989496855707	1.92102671855101	-1.56894464656217
C	3.12562339111973	0.63205402359200	2.07060955247356
H	2.60758344151039	1.04239446240728	2.95427062924974
H	3.93512373087809	-0.03141617176504	2.41662589997030
H	3.60859574243238	1.46488914644741	1.53444513354334

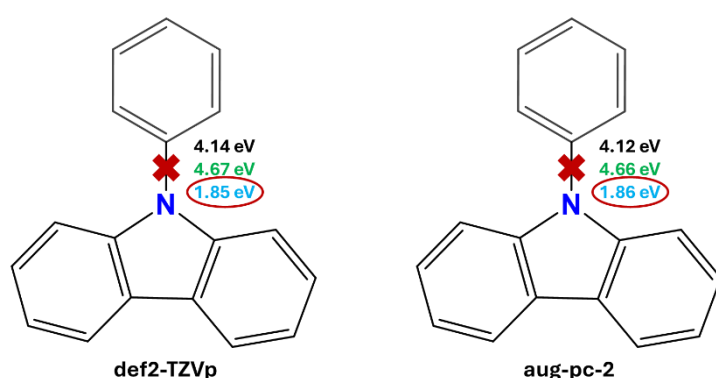


Figure S1 Bond dissociation energies for neutral (black), cationic (green), and anionic (blue) species calculated in def2-TZVp and aug-pc-2 basis sets. For the cationic and anionic forms, the lowest dissociation energy obtained among all cleavage channels is reported.