

ELECTRONIC SUPPLEMENTARY INFORMATION

Improving mobility and stability of electron transport materials for inverted perovskite solar cells by nitrogen substitution

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Table ESII Energies (E , au) of the studied compounds optimized by B3LYP/6-31+g (d, p) in dichloromethane

Compounds	E
TDTP	- 2599.778
TDTP-1	- 2710.484
TDTP-2a	- 2631.866
TDTP-2b	- 2631.876
TDTP-3a	- 2742.570
TDTP-3b	- 2742.583

Table ESI2 The bond length changes (BLC) between TDTP and designed molecules and the sum of absolute value of BLC ($\Sigma|\Delta R|$)

	TDTP	TDTP-1	TDTP-2a	TDTP-2b	TDTP-3a	TDTP-3b
1	0	-0.00066	-0.00052	-0.00062	-0.00053	-0.0005
2	0	9E-05	0.00086	0.00061	0.00088	0.00052
3	0	0.00016	-0.00032	-6E-05	-0.00053	-1E-04
4	0	1E-05	-0.00013	0.00012	-4E-05	9E-05
5	0	0.00012	-5E-05	-7E-05	-2E-05	-3E-05
6	0	6E-05	0.00015	1E-05	0.00021	2E-05
7	0	0.00021	0.00027	0.00018	0.00036	0.00023
8	0	-0.00019	-0.00057	-0.00051	-0.0005	-0.0004
9	0	-0.00012	-0.0014	-0.00056	-0.00183	-0.00071
10	0	-0.00024	0.00376	0.00238	0.00427	0.00227
11	0	-0.0003	0.00159	0.00039	0.00185	0.00056
12	0	-0.00037	-0.0028	-0.00182	-0.00277	-0.00157
13	0	0.00018	-0.0065	-0.00206	-0.00744	-0.00225
14	0	0.00064	-0.00668	-0.00195	-0.00769	-0.00251
15	0	0.00057	-0.00129	-0.0018	-0.00136	-0.00187
16	0	-0.00043	0.0007	-0.00047	0.00105	-0.00011
17	0	0.00051	-0.00051	-0.00016	-0.0006	6E-05
$\Sigma \Delta R $	0	0.005	0.028	0.014	0.032	0.014

Table ESI3 The calculated HOMO level (eV), excitation energies (E_g , eV) and LUMO level of TDTP derivatives

Compounds	HOMO	E_g	LUMO
TDTP	-5.67	1.62	-4.05
TDTP-1	-5.64	1.63	-4.02
TDTP-2a	-6.15	1.93	-4.21
TDTP-2b	-6.13	1.93	-4.19
TDTP-3a	-6.00	1.80	-4.20
TDTP-3b	-5.93	1.78	-4.15

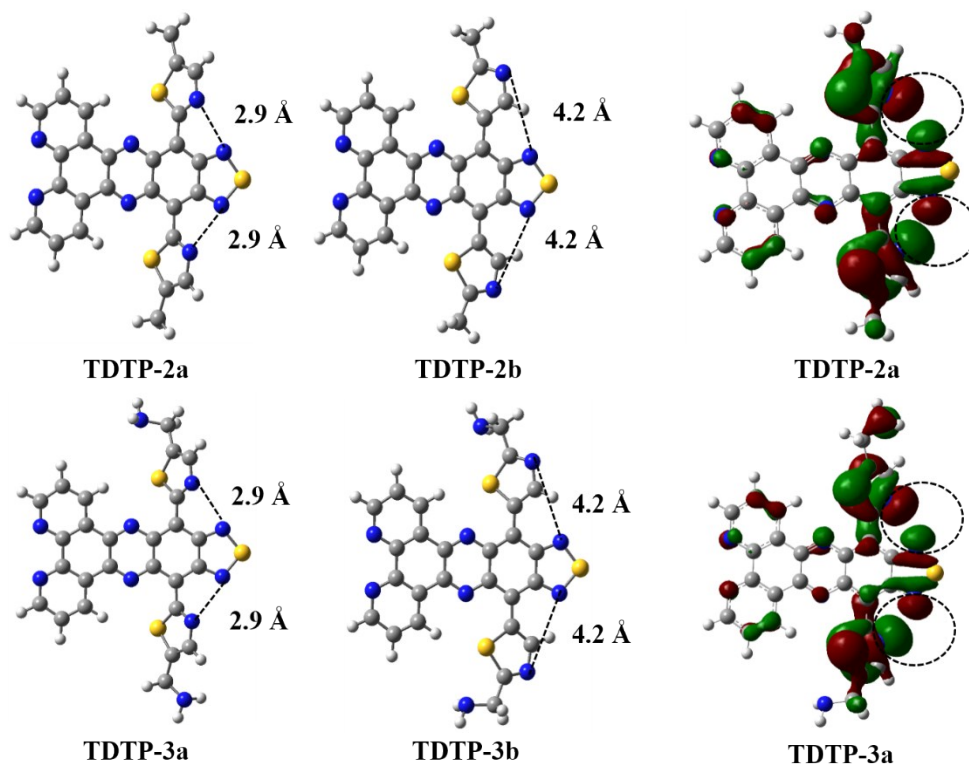


Fig. ESI1 Structure comparison of TDTP-2a, TDTP-2b, TDTP-3a, and TDTP-3b, and the two orbitals with the most contributions of lone pair electrons of nitrogen atoms in thiazole and thiadiazole of TDTP-2a and TDTP-3a.

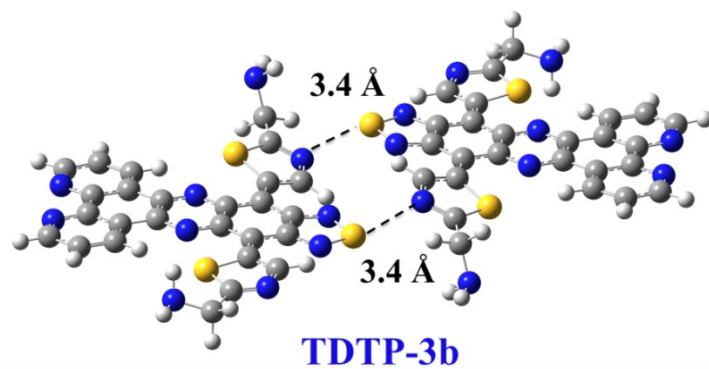


Fig. ESI2 The dimer structure of path 4 in TDTP-3b and the interactions marked by dashed line.

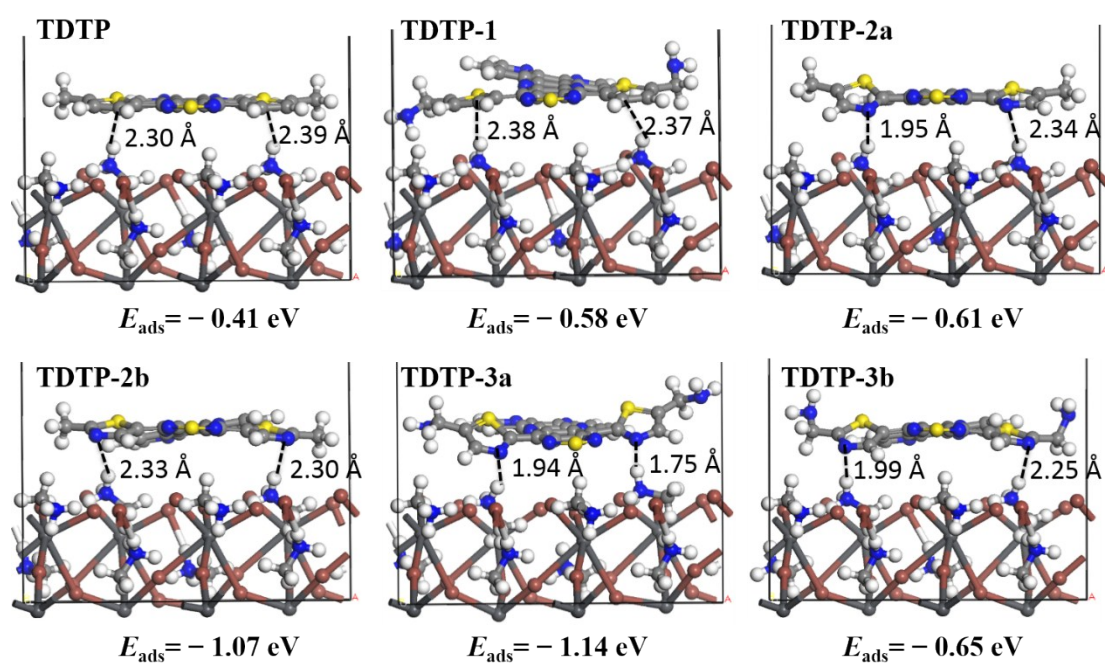


Fig. ES13 The optimized configurations of TDTP-based ETMs adsorbed on the MAI-terminated perovskite surface, together with the corresponding adsorption energy (E_{ads}). The dashed lines indicate the key H...N distances.

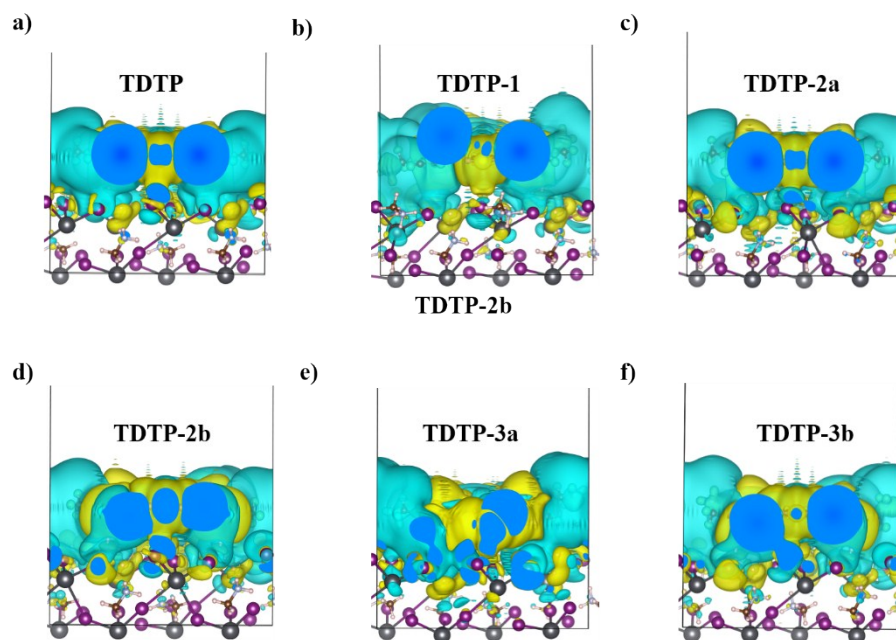


Fig. ESI4 Charge density difference for the TDTP-based ETMs adsorbed on the MAI-terminated perovskite surface, where the yellow color represents charge depletion and the blue color identifies charge accumulation.

Coordinates of the studied compounds optimized by B3LYP/6-31+g (d, p) in dichloromethane

TDTP			TDTP-1				
C	0.73512605	-3.02940023	-0.12941301	C	-0.99307000	-2.90252900	0.02722000
C	1.50290211	-1.82476814	-0.12064701	C	-1.63856300	-1.62900400	0.08985100
C	0.73095006	-0.63266005	-0.10017501	C	-0.75440500	-0.51785500	0.05009200
C	-0.72933206	-0.63442205	-0.10046201	C	0.69143200	-0.66059400	-0.09318500
C	-1.49855911	-1.82831014	-0.11984601	C	1.34101800	-1.92229800	-0.13233100
C	-0.72801205	-3.03113523	-0.12880401	C	0.46107700	-3.04495700	-0.06001000
C	-0.72408906	1.68766713	-0.09858901	C	0.90448400	1.64999500	-0.14790600
C	0.72003006	1.68946213	-0.09667501	C	-0.51212900	1.79038800	0.09349600
C	1.44259211	2.96316023	-0.10446901	C	-1.08912000	3.12543500	0.25824200
C	0.73486905	4.18924632	-0.09105001	C	-0.27925100	4.27790800	0.11463500
C	-0.74546306	4.18732832	-0.09476501	C	1.16021300	4.13483000	-0.20021700
C	-1.44993011	2.95942523	-0.11023801	C	1.73118500	2.84523400	-0.32320100
C	-2.71253021	5.38725543	-0.11228001	C	3.18583400	5.14063700	-0.63888300
C	-3.49889127	4.22573832	-0.13834301	C	3.84279500	3.90909000	-0.78042900
C	-2.85536222	2.99914223	-0.13857601	C	3.10217700	2.74927700	-0.62133900
H	-3.18425024	6.36763947	-0.10963501	H	3.73609100	6.07124000	-0.76059800
H	-4.58123335	4.29566033	-0.15931601	H	4.90209200	3.87545300	-1.01171400
H	-3.41081626	2.06917516	-0.16017801	H	3.55498600	1.76983500	-0.72217800
C	2.84802122	3.00661323	-0.12648201	C	-2.45038100	3.30185500	0.56400900
C	3.48833327	4.23488932	-0.12191101	C	-2.95135500	4.58548200	0.70659200
C	2.69884521	5.39432942	-0.09779801	C	-2.06957100	5.66402300	0.54071000
H	3.40602226	2.07814816	-0.14660701	H	-3.08327000	2.43029900	0.68339200
H	4.57057335	4.30764333	-0.13792001	H	-3.99528400	4.76134300	0.94337800
H	3.16799624	6.37592750	-0.09149501	H	-2.42855100	6.68550200	0.64717300
S	0.00625700	-5.32084840	-0.07547501	S	-0.48850200	-5.25436000	-0.00749300
C	-5.43430141	-1.47769511	0.27599902	C	5.30072400	-1.93130300	-0.03584700
C	-5.15775339	-2.67312020	-0.34569103	C	2.78436800	-2.09482100	-0.24193600
C	-3.77205029	-2.89835122	-0.55556104	S	3.94792400	-0.89971100	0.34074200
C	-2.95546922	-1.86721714	-0.11434301	C	-5.52240600	-0.84657500	-0.02971500
S	-3.96418430	-0.58742904	0.56944004	C	-3.08783300	-1.51741300	0.18249400
H	-5.93004444	-3.37461726	-0.64327205	S	-3.98748500	-0.10159600	-0.37399300
H	-3.37818126	-3.79359029	-1.01471308	N	1.88858900	5.25808800	-0.35845600
C	5.43843142	-1.46581811	0.27052702	N	-0.77578800	5.52320600	0.25529100
C	5.16365439	-2.66137921	-0.35165803	N	1.45651100	0.45712300	-0.21618300
C	3.77815429	-2.88949722	-0.55975604	N	-1.28656700	0.72826000	0.16570900
C	2.95991523	-1.86050714	-0.11660801	N	0.85384600	-4.33442300	-0.06925100
S	3.96674330	-0.57903004	0.56671505	N	-1.62765600	-4.09145900	0.04597700
H	5.93707144	-3.36092726	-0.65090005	C	-5.34964500	-2.10152900	0.50656700
H	3.38562526	-3.78522029	-1.01910908	C	4.87636200	-3.11247900	-0.59905300
C	6.77530852	-0.90130707	0.64925205	H	5.55874300	-3.89006400	-0.92593200
H	6.96748755	0.05686200	0.15325001	H	-6.17896300	-2.72907000	0.80888100
H	6.85280452	-0.73143805	1.72920313	C	-6.80582700	-0.09058300	-0.26381100
H	7.56572460	-1.59841112	0.35806503	H	-7.01474700	0.54359100	0.60777200
C	-6.77188454	-0.91589407	0.65627405	H	-6.67167600	0.59365200	-1.11652600
H	-6.84819952	-0.74554806	1.73623513	C	6.71461800	-1.46611300	0.17188100
H	-6.96688752	0.04155600	0.15998501	H	7.37095900	-2.34391500	0.06973200
H	-7.56118659	-1.61490412	0.36664003	H	6.99357600	-0.76999300	-0.62975300
N	-1.38056511	5.37655843	-0.09352101	N	-7.93886900	-1.01080300	-0.42144900
N	1.36683811	5.38016044	-0.08524501	H	-8.80578400	-0.48103200	-0.46281700
N	-1.39232511	0.55326504	-0.09963701	H	-7.86070500	-1.51770200	-1.30057100
N	1.39106710	0.55668104	-0.09738401	N	6.87107700	-0.74644000	1.44462000
N	-1.24299010	-4.27677633	-0.09789601	H	6.75890600	-1.38623400	2.22839200
N	1.25303310	-4.27384332	-0.09897501	H	7.80925200	-0.35936800	1.51111500
				C	3.46549500	-3.20986900	-0.71064100
				C	-3.98740900	-2.48178700	0.61738600
				H	2.95834100	-4.07520400	-1.11207400
				H	-3.66787100	-3.43919900	1.00241000

TDTP-2a

C	0.73180100	-2.99979600	-0.11543600
C	1.48042200	-1.79120200	-0.13666700
C	0.72892200	-0.59386900	-0.11080700
C	-0.72855600	-0.59430100	-0.11082000
C	-1.47937400	-1.79206800	-0.13655300
C	-0.73005200	-3.00022700	-0.11535300
C	-0.72444300	1.72135400	-0.10013500
C	0.72343300	1.72178800	-0.09994000
C	1.44605600	2.99484400	-0.09953900
C	0.73932900	4.22111800	-0.08726400
C	-0.74187200	4.22066300	-0.08767600
C	-1.44784400	2.99396100	-0.10016400
C	-2.70851100	5.42031300	-0.08825400
C	-3.49629900	4.25940700	-0.10433200
C	-2.85342600	3.03254100	-0.11121700
H	-3.17983600	6.40079400	-0.08263800
H	-4.57865300	4.33041800	-0.11236100
H	-3.40849000	2.10173900	-0.12465300
C	2.85161800	3.03428800	-0.10989200
C	3.49373600	4.26154800	-0.10251300
C	2.70523200	5.42197200	-0.08663500
H	3.40725900	2.10382900	-0.12316700
H	4.57605000	4.33322100	-0.10999200
H	3.17595700	6.40273900	-0.08059900
S	0.00155700	-5.27664900	0.03844600
C	-5.37943100	-1.58172200	0.20468400
C	-4.97981600	-2.57574600	-0.65528400
C	-2.94469000	-1.82784300	-0.17281200
S	-3.96625200	-0.74365600	0.77530400
H	-5.66346300	-3.23790800	-1.17510200
C	5.38041400	-1.57878400	0.20406400
C	4.98121500	-2.57288700	-0.65600300
C	2.94575500	-1.82617200	-0.17310600
S	3.96685800	-0.74158800	0.77503800
H	5.66514600	-3.23458900	-1.17603300
N	-1.37615900	5.40965600	-0.08098600
N	1.37288100	5.41050700	-0.08005200
N	-1.39782300	0.59168800	-0.11212900
N	1.39749000	0.59252200	-0.11192000
N	-1.25237100	-4.24108800	-0.03106300
N	1.25486600	-4.24034600	-0.03121300
N	3.63323400	-2.71483900	-0.85407500
N	-3.63179000	-2.71699100	-0.85353600
C	6.77243500	-1.19974300	0.60789200
H	7.49022300	-1.85127900	0.10220800
H	7.00347200	-0.16355800	0.33815100
H	6.92236900	-1.30146800	1.68812400
C	-6.77160100	-1.20337900	0.60865800
H	-7.00327500	-0.16738800	0.33871700
H	-7.48910300	-1.85543900	0.10324500
H	-6.92129400	-1.30494000	1.68893900

TDTP-2b

C	-0.73097600	-3.02698700	-0.00919900
C	-1.49541200	-1.82284300	-0.03614000
C	-0.72858500	-0.62971000	-0.03244800
C	0.72843000	-0.62988600	0.03244300
C	1.49497200	-1.82320100	0.03613200
C	0.73024700	-3.02716300	0.00918300
C	0.71912800	1.69000000	0.07900500
C	-0.71871600	1.69017500	-0.07900800
C	-1.43152400	2.96181000	-0.21086500
C	-0.73062900	4.18821400	-0.11720800
C	0.73164900	4.18803600	0.11720800
C	1.43224600	2.96146000	0.21086300
C	2.66911600	5.39024300	0.44669300
C	3.44972500	4.23007400	0.56000700
C	2.81895600	3.00262800	0.44171200
H	3.13089000	6.37119900	0.53611100
H	4.51707000	4.30167600	0.73956900
H	3.37038400	2.07393500	0.52632500
C	-2.81822500	3.00331600	-0.44171600
C	-3.44869300	4.23091600	-0.56001300
C	-2.66780200	5.39089400	-0.44669700
H	-3.36987900	2.07475900	-0.52633200
H	-4.51602000	4.30277900	-0.73957700
H	-3.12933600	6.37196300	-0.53611700
S	-0.00064400	-5.31717400	-0.00001000
C	5.39801700	-1.52291600	-0.18076000
C	3.77468700	-2.89390400	-0.45232500
C	2.95111600	-1.85142400	0.06358200
S	3.98547200	-0.54112500	-0.49714300
H	3.41251100	-3.83228000	0.84513500
C	-5.39839200	-1.52171900	0.18078400
C	-3.77535700	-2.89303900	-0.45233700
C	-2.95156300	-1.85073800	-0.06359100
S	-3.98563700	-0.54022500	0.49715500
H	-3.41338200	-3.83149100	-0.84515200
N	1.35395400	5.37771900	0.23395900
N	-1.35264300	5.37804900	-0.23396100
N	1.38848000	0.55733600	0.11028800
N	-1.38834400	0.55767400	-0.11029300
N	1.24745600	-4.27173900	0.00264100
N	-1.24848900	-4.27143600	-0.00267000
N	-5.12597100	-2.70219000	-0.32363600
N	5.12534200	-2.70333600	0.32364100
C	-6.78468300	-1.01451600	0.43032000
H	-7.02129800	-0.16872100	-0.22463200
H	-7.49661000	-1.81855900	0.23269100
H	-6.90833900	-0.67691000	1.46427000
C	6.78441800	-1.01599700	-0.43026800
H	7.02119600	-0.17025800	0.22469700
H	7.49617500	-1.82018900	-0.23263500
H	6.90816000	-0.67840600	-1.46421200

TDTP-3a

C	1.13610700	-2.80609000	-0.16845600
C	1.69916200	-1.50065800	-0.17182100
C	0.78080700	-0.42620400	-0.14376100
C	-0.66086200	-0.64050300	-0.14746600
C	-1.22665200	-1.93477300	-0.18076200
C	-0.30989600	-3.02022800	-0.17365200
C	-0.99720600	1.64975500	-0.12919300
C	0.43540100	1.86299700	-0.12803900
C	0.96271400	3.22846900	-0.12790400
C	0.08286200	4.33713200	-0.11584500
C	-1.38220600	4.11899100	-0.11400300
C	-1.90004800	2.80200100	-0.12569000
C	-3.50362400	5.01625900	-0.10924700
C	-4.11220800	3.75206200	-0.12244500
C	-3.29607100	2.63293200	-0.13160600
H	-4.11409600	5.91667900	-0.10241200
H	-5.19323200	3.66314800	-0.12596000
H	-3.70809900	1.63049400	-0.14225500
C	2.34717500	3.47481100	-0.13949800
C	2.80119200	4.78336400	-0.13383100
C	1.85022100	5.81476600	-0.11830500
H	3.03377800	2.63624400	-0.15287200
H	3.86107000	5.01404500	-0.14257600
H	2.17109200	6.85424000	-0.11385700
S	0.74619100	-5.16734700	-0.05089200
C	-5.10523500	-2.30656500	0.18704000
C	-2.67310000	-2.18398000	-0.20932800
S	-3.82161900	-1.30573200	0.79874900
C	5.51670200	-0.72301700	0.22294500
C	3.15426200	-1.31993600	-0.19143800
S	3.99161600	-0.11701600	0.79362100
N	-2.18414600	5.20208900	-0.10561300
N	0.53407300	5.60685300	-0.11032400
N	-1.49776300	0.43411900	-0.14579000
N	1.26834800	0.84542900	-0.14058200
N	-0.64561300	-4.32552100	-0.10959200
N	1.83464200	-3.95833300	-0.09998900
C	5.28471900	-1.74980400	-0.65942900
C	-4.58345800	-3.18441100	-0.73069900
N	3.97278300	-2.08446900	-0.87687300
N	-3.23050100	-3.12368600	-0.94027200
H	-5.17296800	-3.90593600	-1.28546000
H	6.06603200	-2.29172200	-1.17613000
C	6.83042600	-0.12424800	0.65550200
H	6.97917000	0.82905100	0.13313400
H	6.78200800	0.11617500	1.72898700
C	-6.53039700	-2.17651100	0.64135700
H	-7.12962900	-2.87807600	0.04148800
H	-6.61459400	-2.50056000	1.68551200
N	7.94760100	-1.00661200	0.30107500
H	8.82720400	-0.52213500	0.45849800
H	7.95315700	-1.82937300	0.90006300
N	-6.99912000	-0.78294800	0.57622700
H	-7.07612200	-0.48348600	-0.39373000
H	-7.93061900	-0.71537900	0.97948200

TDTP-3b

C	0.65884100	-3.05254700	-0.00049900
C	1.44929100	-1.86670700	0.05603400
C	0.71176300	-0.65583400	0.02318600
C	-0.74228900	-0.62255600	-0.08839900
C	-1.53500700	-1.79797600	-0.12077000
C	-0.80034000	-3.01914200	-0.07105600
C	-0.67898400	1.69618400	-0.12827500
C	0.75412600	1.66333300	0.06452800
C	1.49410000	2.91857400	0.20460600
C	0.82342500	4.16065800	0.09836500
C	-0.63462900	4.19414400	-0.15833100
C	-1.36081400	2.98396200	-0.26834700
C	-2.53960800	5.44050900	-0.51164600
C	-3.34410700	4.29849200	-0.64120400
C	-2.74279800	3.05671100	-0.51878000
H	-2.97816700	6.43185700	-0.60343700
H	-4.40702500	4.39451400	-0.83501600
H	-3.31374000	2.14071300	-0.61315400
C	2.87843100	2.92809200	0.45230300
C	3.53556600	4.14093600	0.57736800
C	2.78328300	5.31851700	0.45309800
H	3.40749100	1.98696900	0.54261800
H	4.60211900	4.18833500	0.76916100
H	3.26626000	6.28875500	0.54764900
S	-0.12304700	-5.32507600	-0.04198200
C	-5.42486900	-1.42932000	-0.02363100
C	-3.81506900	-2.80433700	-0.66237400
C	-2.99021800	-1.79255500	-0.20114300
S	-4.01432400	-0.48608600	0.38709400
H	-3.45642600	-3.73275400	-1.08203000
C	5.35435600	-1.67837700	0.00249700
C	3.67466300	-2.98382400	0.60589600
C	2.90317600	-1.93277100	0.13978000
S	3.99477600	-0.66664000	-0.41475900
H	3.26852900	-3.89463900	1.02064800
N	-1.22835900	5.39806600	-0.27919300
N	1.47123300	5.33599000	0.22225900
N	-1.37303800	0.57953800	-0.18234100
N	1.39664200	0.51617000	0.11752900
N	-1.34659600	-4.25156900	-0.08575100
N	1.14802000	-4.30883000	0.00757600
N	5.03394400	-2.83019400	0.54016500
N	-5.16485400	-2.59417400	-0.56595600
C	6.76932700	-1.23875300	-0.25867900
H	7.08747800	-1.66218600	-1.21965200
H	7.40593000	-1.69299000	0.51426400
C	-6.81364000	-0.88318900	0.16553800
H	-7.13763500	-0.42963600	-0.77965500
H	-7.48134700	-1.73664800	0.35235800
N	-6.84301300	0.15654400	1.19679100
H	-7.70857200	0.68504200	1.13904100
H	-6.80608100	-0.25476000	2.12644300
N	6.86758200	0.21972500	-0.35558600
H	6.84324800	0.64523400	0.56820700
H	7.75066100	0.48479800	-0.78192500