

Supporting Information for:
**The origin of regio- and stereoselectivity in 1,3-dipolar cycloaddition
of nitrile oxides with C₁-substituted 7-oxabenzonorbornadienes, A
DFT study**

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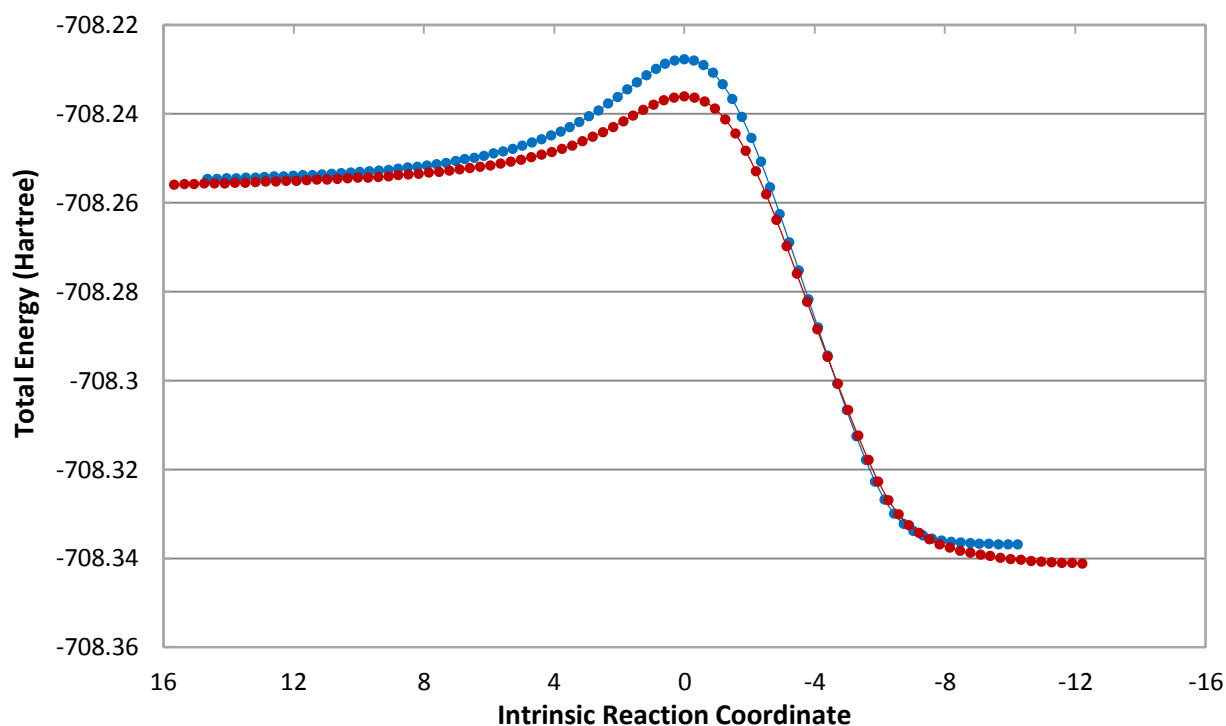


Figure S1. B3LYP/6-31G(d) IRC plot for the reaction pathways leading to **3X (ba)** and **3N (ba)**.

Table S1. B3LYP/6-31G(d) HOMO and LUMO energies, electronic chemical potential, μ , chemical hardness, η , electrophilicity, ω , and nucleophilicity, N^a , indices, in eV, of the reactants

Reactants	ϵ_{HOMO}	ϵ_{LUMO}	μ	η	ω	N^a
1a	-6.73	0.94	-2.89	7.66	0.55	2.39
1b	-6.34	-1.31	-3.82	5.02	1.46	2.78
2a	-5.98	-0.53	-3.25	5.45	0.97	3.15
2b	-5.92	-0.50	-3.21	5.41	0.95	3.20
2c	-5.88	-0.46	-3.17	5.42	0.93	3.25
2d	-6.17	-0.71	-3.44	5.45	1.08	2.95

^a HOMO energy of tetracyanoethylene is -9.12 eV at the same level of theory.

Table S2. Electronic energies (E), sum of electronic and zero-point energies (E_{zpv}), sum of electronic and thermal enthalpies (H), sum of electronic and thermal Gibbs energies (G), in a. u., and entropies (S), in Cal mol⁻¹ K⁻¹, for the all species at B3LYP/6-31G(d) level of theory

	E	E_{zpv}	H	G	S
1a	-207.899238	-207.849444	-207.843747	-207.875943	67.763
1b	-399.639891	-399.536429	-399.528207	-399.569137	86.145
2a	-461.030900	-460.878648	-460.870557	-460.910430	83.921
2b	-500.352421	-500.172707	-500.162984	-500.206110	90.765
2c	-869.704174	-869.450998	-869.434677	-869.493168	123.104
2d	-613.675175	-613.486445	-613.474545	-613.523727	103.514
TSXA (aa)	-668.913927	-668.710857	-668.697589	-668.750151	110.625
TSNA (aa)	-668.906136	-668.703145	-668.690044	-668.741746	108.817
TSXA (ab)	-860.654676	-860.398104	-860.382085	-860.442356	126.851
TSNA (ab)	-860.646311	-860.389959	-860.373992	-860.434145	126.602
TSXA (ba)	-708.236044	-708.005543	-707.990646	-708.046292	117.117
TSNA (ba)	-708.227731	-707.997293	-707.982519	-708.037498	115.714
TSXS (ba)	-708.233609	-708.002960	-707.988103	-708.043793	117.209
TSNS (ba)	-708.227438	-707.997034	-707.982262	-708.037206	115.639
TSXA (bb)	-899.976701	-899.692587	-899.674954	-899.738322	133.368
TSNA (bb)	-899.967895	-899.684111	-899.666482	-899.729532	132.701
TSXS (bb)	-899.974207	-899.690159	-899.672529	-899.735810	133.185
TSNS (bb)	-899.967660	-899.683867	-899.666251	-899.729290	132.676
TSXA (ca)	-1077.587053	-1077.282806	-1077.261411	-1077.331565	147.651
TSNA (ca)	-1077.579236	-1077.275547	-1077.254044	-1077.324590	148.476
TSXS (ca)	-1077.580977	-1077.276785	-1077.255461	-1077.325198	146.774
TSNS (ca)	-1077.578618	-1077.274710	-1077.253334	-1077.323344	147.348
TSXA (da)	-821.559786	-821.320107	-821.303130	-821.363898	127.898
TSNA (da)	-821.548264	-821.308902	-821.291881	-821.353601	129.900
TSXS (da)	-821.559228	-821.319476	-821.302492	-821.363571	128.551
TSNS (da)	-821.554128	-821.314294	-821.297570	-821.357319	125.752
3X (aa)	-669.019108	-668.810311	-668.798583	-668.846941	101.778
3N (aa)	-669.015165	-668.806292	-668.794623	-668.842800	101.397
3X (ab)	-860.758842	-860.496637	-860.481887	-860.538313	118.758
3N (ab)	-860.755156	-860.492838	-860.478156	-860.534347	118.262
3X (ba)	-708.341186	-708.104813	-708.091466	-708.142923	108.299
3N (ba)	-708.336915	-708.100648	-708.087296	-708.138737	108.267
4X (ba)	-708.338168	-708.101612	-708.088346	-708.139567	107.804
4N (ba)	-708.336445	-708.100120	-708.086791	-708.138137	108.066
3X (bb)	-900.080882	-899.791072	-899.774696	-899.834194	125.223
3N (bb)	-900.076898	-899.787161	-899.770800	-899.830308	125.246
4X (bb)	-900.077786	-899.787856	-899.771599	-899.830583	124.142
4N (bb)	-900.075599	-899.785804	-899.769502	-899.828787	124.776
3X (ca)	-1077.693936	-1077.383921	-1077.364067	-1077.429989	138.745
3N (ca)	-1077.688238	-1077.378527	-1077.358519	-1077.425280	140.512
4X (ca)	-1077.686545	-1077.376317	-1077.356579	-1077.421885	137.449
4N (ca)	-1077.687100	-1077.377102	-1077.357296	-1077.423433	139.197
3X (da)	-821.663883	-821.418398	-821.402941	-821.459621	119.294
3N (da)	-821.656309	-821.411047	-821.395519	-821.452766	120.487
4X (da)	-821.662018	-821.416615	-821.401089	-821.458218	120.237
4N (da)	-821.659819	-821.414413	-821.398907	-821.456054	120.276

Table S3. Single point energies (E), enthalpies (H)^a and Gibbs energies (G)^a for reactants and TSs, at M05-2X(UF)/6-311++G(2d,2p)//B3LYP/6-31G(d), in a. u.

Structure	E	H	G
1a	-207.928534	-207.873043	-207.905239
1b	-399.706620	-399.594936	-399.635866
2a	-461.127487	-460.967144	-461.007017
2b	-500.455385	-500.265947	-500.309073
2c	-869.828503	-869.559006	-869.617497
2d	-613.804187	-613.603557	-613.652739
TSXA (aa)	-669.038522	-668.822184	-668.874746
TSNA (aa)	-669.032445	-668.816353	-668.868055
TSXA (ab)	-860.817374	-860.544783	-860.605054
TSNA (ab)	-860.810986	-860.538666	-860.598819
TSXA (ba)	-708.367216	-708.121818	-708.177464
TSNA (ba)	-708.360690	-708.115478	-708.170457
TSXS (ba)	-708.364801	-708.119295	-708.174985
TSNS (ba)	-708.360714	-708.115538	-708.170482
TSXA (bb)	-900.145922	-899.844175	-899.907543
TSNA (bb)	-900.139225	-899.837812	-899.900862
TSXS (bb)	-900.144068	-899.842389	-899.905670
TSNS (bb)	-900.139876	-899.838467	-899.901506
TSXA (ca)	-1077.739312	-1077.413670	-1077.483824
TSNA (ca)	-1077.733794	-1077.408603	-1077.479149
TSXS (ca)	-1077.734576	-1077.409061	-1077.478798
TSNS (ca)	-1077.733950	-1077.408666	-1077.478676
TSXA (da)	-821.716868	-821.460212	-821.520980
TSNA (da)	-821.706854	-821.450471	-821.512191
TSXS (da)	-821.717392	-821.460656	-821.521735
TSNS (da)	-821.713710	-821.457152	-821.516901

^a Calculated as the sum of M05-2X(UF)/6-311++G(2d,2p) energies and the thermal corrections to enthalpies or Gibbs energies obtained from thermochemical calculations (298.15 K, 1 atm) at the B3LYP/6-31G(d) level.

Table S4. Some of dihedral angle values, in degree, at the optimized reactants and TSs

Structures	θ_1	θ_2	θ_3	θ_4	θ_5	θ_6
2a	-174.7	174.7	151.5	-151.5	30.4	-30.4
2b	-174.9	174.6	152.0	-151.5	30.5	-30.4
2c	-175.0	174.2	153.0	-151.5	34.8	-30.2
2d	-174.7	174.0	152.0	-151.7	27.5	-30.8
TSXA (aa)	-155.6	160.5	164.8	-170.4	43.7	-49.9
TSNA (aa)	153.9	-162.1	128.6	-119.9	8.9	0.1
TSXA (ab)	-155.3	160.6	164.7	-170.9	43.6	-50.5
TSNA (ab)	153.4	-162.5	128.8	-119.2	9.2	0.7
TSXA (ba)	-155.4	160.5	165.2	-170.8	43.1	-50.1
TSNA (ba)	153.7	-162.2	129.4	-119.9	9.1	0.2
TSXS (ba)	-159.6	153.5	172.9	-165.9	51.1	-44.6
TSNS (ba)	161.7	-154.0	120.8	-128.5	0.4	-8.7
TSXA (bb)	-155.1	160.5	165.3	-171.4	43.1	-50.8
TSNA (bb)	153.3	-162.7	129.7	-119.2	9.4	0.7
TSXS (bb)	-159.5	153.5	173.1	-166.0	51.2	-44.8
TSNS (bb)	161.9	-153.3	119.9	-128.4	-0.4	-8.7

TSXA (ca)	-154.5	159.3	167.1	-172.2	46.6	-51.2
TSNA (ca)	153.3	-162.9	130.2	-119.5	13.5	0.8
TSXS (ca)	-159.2	151.1	175.9	-166.6	56.8	-45.1
TSNS (ca)	160.6	-154.9	121.6	-127.4	6.0	-7.4
TSXA (da)	-154.7	160.6	164.2	-171.3	39.9	-51.0
TSNA (da)	152.4	-162.8	130.0	-118.9	7.2	1.0
TSXS (da)	-160.7	152.7	172.4	-164.9	48.2	-44.1
TSNS (da)	162.2	-152.7	119.6	-128.8	-3.8	-9.3

Cartesian coordinates for all optimized reactants, transition states and products at B3LYP/6-31G(d) level

1a

C	0.43007600	0.00052300	-0.00015300
N	-0.73502300	0.00023400	-0.00008400
C	1.89122900	-0.00021700	0.00006800
H	2.28065500	1.00186000	-0.21256600
H	2.27984300	-0.31735700	0.97445100
H	2.27986900	-0.68574700	-0.76152200
O	-1.95287900	-0.00027900	0.00009300

1b

C	1.47288300	-0.00008900	-0.00004300
N	2.64140700	0.00000000	-0.00001200
O	3.85693900	0.00003100	0.00004300
C	0.04520300	-0.00004900	-0.00002200
C	-0.66434300	1.21651900	-0.00001300
C	-0.66442700	-1.21655600	-0.00001200
C	-2.05632500	1.20931000	0.00001000
H	-0.11669400	2.15357300	-0.00002200
C	-2.05641800	-1.20924700	0.00001000
H	-0.11685800	-2.15365700	-0.00002100
C	-2.75594800	0.00005300	0.00002100
H	-2.59659300	2.15173600	0.00001900
H	-2.59674200	-2.15164000	0.00001800
H	-3.84222700	0.00009900	0.00003800

2a

C	-2.58694600	0.69598800	0.16303500
C	-2.58694700	-0.69598500	0.16303400
C	-1.38694200	-1.41894100	0.00639900
C	-0.21782300	-0.70305200	-0.15376500
C	-0.21782200	0.70305100	-0.15376500
C	-1.38694000	1.41894200	0.00640000
C	1.26314500	-1.07322000	-0.34737400
C	1.99756300	-0.66706900	0.94741000

C	1.99756700	0.66707100	0.94740500
C	1.26314600	1.07321800	-0.34737800
O	1.66805100	-0.00000300	-1.22816500
H	-3.52389900	1.23405700	0.28026000
H	-3.52390100	-1.23405300	0.28026000
H	-1.39616800	-2.50627000	0.00525100
H	-1.39616500	2.50627100	0.00525100
H	1.49138700	-2.04670000	-0.78091600
H	2.34247200	-1.35037500	1.71387300
H	2.34248000	1.35038100	1.71386400
H	1.49138800	2.04669600	-0.78092400

2b

C	-2.57405700	1.04461700	0.26323500
C	-2.89908300	-0.28331700	0.00290500
C	-1.89215800	-1.23657400	-0.25241100
C	-0.58006600	-0.80889700	-0.24315200
C	-0.25060800	0.53214700	0.01932300
C	-1.22987900	1.47012400	0.27808400
C	0.78278000	-1.48706400	-0.45904300
C	1.49467700	-1.50328200	0.90899600
C	1.80174400	-0.22955900	1.15658400
C	1.29185000	0.57683800	-0.06350900
O	1.49017700	-0.41160300	-1.11213000
H	-3.36523300	1.76510200	0.45359100
H	-3.94162400	-0.59022700	-0.00807900
H	-2.15420400	-2.27193700	-0.45694300
H	-0.98649700	2.51038900	0.48063800
H	0.80688800	-2.39760000	-1.05786700
H	1.61324700	-2.37138800	1.54627300
H	2.23816000	0.20655600	2.04769300
C	1.96495400	1.88861000	-0.39206900
H	1.80226500	2.61537000	0.41163500
H	3.04267600	1.74191300	-0.51233100
H	1.56197400	2.30278600	-1.32122300

2c

C	2.66934400	-1.95942600	0.32630400
C	3.60598800	-1.03144100	-0.11717000
C	3.21808400	0.28637400	-0.43333700
C	1.88573500	0.61981700	-0.30013000
C	0.93330100	-0.31741500	0.14232200
C	1.31137400	-1.60657900	0.46582000
C	1.07305900	1.90457000	-0.51712000
C	0.63559500	2.38893000	0.87888700
C	-0.26417500	1.49616800	1.29474300
C	-0.40889400	0.45740900	0.15049400
O	-0.15923900	1.33494700	-1.00061500
H	2.98499900	-2.97161800	0.56539800
H	4.64722300	-1.32412300	-0.22356800

H	3.95491800	1.00875100	-0.77680200
H	0.59287300	-2.34319900	0.81651100
H	1.46923700	2.64378900	-1.21401800
H	1.06567900	3.22555700	1.41660600
H	-0.74813500	1.42869200	2.26222600
Si	-2.08269700	-0.43999000	-0.09738300
C	-3.39913900	0.88597600	-0.37113800
H	-3.13409300	1.51748200	-1.22592100
H	-4.38020400	0.43752000	-0.56941300
H	-3.50133500	1.53924600	0.50331800
C	-1.94711400	-1.56622200	-1.60740600
H	-1.18530300	-2.34133200	-1.46749100
H	-2.90075800	-2.06546200	-1.81794900
H	-1.66763300	-0.98517200	-2.49334700
C	-2.48433000	-1.44447900	1.45975100
H	-3.46095700	-1.93343200	1.35571600
H	-1.74484600	-2.23030200	1.65319800
H	-2.53296600	-0.80820100	2.35169200

2d

C	2.41129100	-1.77817900	0.17143400
C	3.20390700	-0.69963400	-0.21289000
C	2.63640900	0.56838500	-0.45095800
C	1.27011200	0.70153900	-0.30349300
C	0.47508800	-0.39095500	0.07859300
C	1.01839100	-1.63359500	0.33031600
C	0.27314500	1.86467900	-0.43378000
C	-0.22523900	2.18902900	0.99049600
C	-0.98086900	1.15046100	1.34771800
C	-0.95655000	0.19304500	0.13348900
O	-0.87019800	1.14572700	-0.95345800
H	2.87099300	-2.74622800	0.35136300
H	4.27554600	-0.83538400	-0.33158700
H	3.26380200	1.40580100	-0.74636500
H	0.39849300	-2.46997000	0.63997700
H	0.54210800	2.69690600	-1.08375200
H	0.08026600	3.04408400	1.58109500
H	-1.45641800	0.91886400	2.29191600
C	-2.09785200	-0.79597600	0.00382600
O	-2.29242500	-1.58232100	0.91330500
C	-2.91831200	-0.75619500	-1.26164400
H	-2.26980900	-0.90480200	-2.13296900
H	-3.69027500	-1.52701200	-1.22448800
H	-3.37085300	0.23486900	-1.38259600

TSXA (aa)

C	-3.72761000	1.01462100	-0.24890100
C	-3.91311800	-0.36505200	-0.22859500
C	-2.82768400	-1.23686100	-0.00966500
C	-1.58043600	-0.67980400	0.19242400

C	-1.39259100	0.71424500	0.16918100
C	-2.44938700	1.57481800	-0.05156600
C	-0.17139600	-1.24139600	0.44534800
C	0.62900600	-0.97275500	-0.83509100
C	0.85190700	0.37763000	-0.84599800
C	0.11457900	0.89038000	0.41375200
O	0.35263300	-0.21009200	1.31469400
O	2.73374300	-1.80566900	-0.13343800
N	3.24353400	-0.69119200	-0.02954500
C	3.06496600	0.49169800	-0.15769900
C	3.68812400	1.81700200	0.00523300
H	-4.57902100	1.66963600	-0.41405200
H	-4.90798900	-0.77639500	-0.37759900
H	-2.98145100	-2.31314400	0.00722300
H	-2.31442500	2.65384400	-0.06723700
H	0.71164300	-1.66615200	-1.66021300
H	1.04246000	0.98202000	-1.72573700
H	0.44326800	1.83272700	0.85315800
H	4.74335000	1.71482400	0.28095100
H	3.18222000	2.39139500	0.78980000
H	3.62858500	2.39292800	-0.92480600
H	-0.08254200	-2.22439700	0.90474100

TSNA (aa)

C	-2.35775900	-1.61253300	-0.46151400
C	-2.68635000	-1.00850200	0.75156100
C	-2.05082200	0.17588200	1.16516600
C	-1.09742400	0.72546300	0.32873600
C	-0.75601800	0.11086800	-0.88690000
C	-1.37515700	-1.05553300	-1.30011600
C	-0.22831900	1.98534300	0.36939900
C	1.24577200	1.58065400	0.56538300
C	1.59456200	0.93205700	-0.58982100
C	0.31790200	1.02665600	-1.47456800
O	-0.20710500	2.31307000	-1.04853700
C	1.82700900	-1.22007200	0.13127500
N	1.53703300	-1.05564300	1.29193100
O	1.19695500	-0.20170100	2.11355700
C	2.20370400	-2.25899100	-0.84494100
H	-2.87311400	-2.51909100	-0.76797300
H	-3.45145800	-1.45298100	1.38252000
H	-2.31284400	0.64032500	2.11206900
H	-1.13116800	-1.52565300	-2.25052900
H	1.89139300	1.97714300	1.33441400
H	2.59386600	0.85095000	-1.00077400
H	0.46765600	1.00564300	-2.55420500
H	2.43438900	-3.19984000	-0.33390700
H	3.08495400	-1.95247700	-1.41877700
H	1.38401400	-2.43956100	-1.54975000
H	-0.58830400	2.82633200	0.96126900

TSXA (ab)

C	-4.31352400	-2.06107200	0.04992100
C	-5.01793300	-0.86136000	-0.00523800
C	-4.34334400	0.36609500	-0.16111400
C	-2.96674700	0.33915600	-0.26674500
C	-2.25470700	-0.87284600	-0.20857000
C	-2.90767900	-2.07881900	-0.04861900
C	-1.87166400	1.40678800	-0.42830300
C	-1.12372400	1.45353500	0.91000200
C	-0.39944300	0.29315900	0.95964100
C	-0.78379500	-0.44869800	-0.34249100
O	-0.92665800	0.67199000	-1.23969100
O	0.52908100	3.02915700	0.31955200
N	1.44268500	2.21284200	0.25980000
C	1.73511000	1.04684000	0.39650300
H	-4.85348200	-2.99714000	0.16579100
H	-6.10227000	-0.87028000	0.06746200
H	-4.90116200	1.29841200	-0.20531200
H	-2.36586800	-3.02077800	-0.00633400
H	-1.37465500	2.11372300	1.72857400
H	-0.06099000	-0.19710700	1.86493400
H	-0.07950200	-1.17949000	-0.73928700
H	-2.13863200	2.35317600	-0.89568400
C	2.81571000	0.11682300	0.18471700
C	3.87006500	0.43811200	-0.69473600
C	2.82734500	-1.12529800	0.84218000
C	4.91023900	-0.46323800	-0.89562300
H	3.85882100	1.39408700	-1.20832700
C	3.87027800	-2.02390600	0.62765300
H	2.02024000	-1.37840800	1.52174100
C	4.91467900	-1.69730900	-0.23880400
H	5.71921500	-0.20322800	-1.57274300
H	3.86777800	-2.98044400	1.14277800
H	5.72713500	-2.39936900	-0.40333000

TSNA (ab)

C	1.31628400	2.76382500	-0.64482400
C	2.35684100	2.68103900	0.28024300
C	2.94853100	1.44471600	0.59352600
C	2.47442300	0.31875500	-0.05375500
C	1.42326700	0.40077700	-0.98063100
C	0.82862900	1.61166000	-1.28678800
C	2.84761000	-1.16522500	-0.04138800
C	1.70714600	-1.97202400	0.61199900
C	0.65476800	-1.87760700	-0.26003800
C	1.22454200	-1.04326700	-1.44392700
O	2.60699700	-1.49044900	-1.43913000
C	-0.83335900	-0.58144200	0.91126600
N	-0.15270000	-0.39061900	1.89787800

O	0.93689300	-0.63986600	2.40722200
H	0.87954000	3.73149000	-0.87741100
H	2.72073800	3.58508600	0.76131300
H	3.75627500	1.38731300	1.31839300
H	0.01376100	1.68270100	-2.00302100
H	1.83884400	-2.66440200	1.43009200
H	-0.14691900	-2.59798100	-0.36793800
H	0.76859000	-1.20313400	-2.42130700
H	3.86290700	-1.42843900	0.25363800
C	-2.14338700	-0.27212200	0.39204500
C	-2.51126600	-0.65916900	-0.90733600
C	-3.07578100	0.42299300	1.19005700
C	-3.78043900	-0.35773400	-1.39780100
H	-1.80157500	-1.19429900	-1.52908900
C	-4.33889000	0.71963600	0.69000800
H	-2.79366800	0.72361000	2.19396200
C	-4.69818700	0.33132500	-0.60418900
H	-4.05100900	-0.66334800	-2.40463100
H	-5.04744400	1.25660900	1.31468700
H	-5.68664300	0.56482800	-0.98936300

TSXA (ba)

C	3.71672400	-1.26049800	-0.17529500
C	3.90858000	0.10664500	-0.35383900
C	2.82901900	1.00713500	-0.25110300
C	1.58062400	0.49302300	0.03955500
C	1.38753800	-0.88792000	0.21666000
C	2.43735500	-1.77815200	0.11176600
C	0.17763400	1.11420400	0.23095600
C	-0.62686000	0.65255300	-0.99903500
C	-0.85796100	-0.68358800	-0.82008800
C	-0.11714600	-1.01775500	0.49490400
O	-0.34407600	0.19605100	1.23388700
O	-2.79515100	1.56157400	-0.48014900
N	-3.27537900	0.46212300	-0.20495900
C	-3.06092900	-0.71981900	-0.13797500
C	-3.65466500	-2.01993300	0.22083200
H	4.56298600	-1.93788400	-0.25419000
H	4.90349700	0.48680900	-0.57041500
H	2.98919800	2.07374200	-0.38882300
H	2.29620700	-2.84744800	0.25164900
H	-0.71099900	1.22284400	-1.91401200
H	-1.04940400	-1.40359200	-1.60833500
H	-0.44661200	-1.88937800	1.06184700
H	-4.71339900	-1.90213900	0.47578300
H	-3.14003100	-2.45757500	1.08388600
H	-3.57651300	-2.72769700	-0.61186300
C	0.07614000	2.55234500	0.67716400
H	0.65254400	2.70937200	1.59411300
H	0.46837200	3.21989200	-0.09834300

H	-0.97070900	2.80775900	0.85650700
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TSNA (ba)

C	-0.40081500	2.96419800	-0.24451500
C	0.48563000	2.82360600	0.82230300
C	1.19958700	1.62729500	1.01589400
C	1.00212000	0.59909400	0.11276400
C	0.09888300	0.73563800	-0.95293600
C	-0.60901200	1.90788800	-1.15021200
C	1.60828000	-0.80330000	-0.06170400
C	0.50523700	-1.84727300	0.23449600
C	-0.41974100	-1.70824100	-0.76443700
C	0.18354200	-0.60512200	-1.68011900
O	1.60008700	-0.87277000	-1.52472700
C	-2.19834500	-0.82871200	0.36417500
N	-1.70461000	-0.76602100	1.46438500
O	-0.67320500	-0.99787600	2.09903000
C	2.98242700	-1.06847800	0.50563100
C	-3.42839500	-0.51444500	-0.38594200
H	-0.93097500	3.90279800	-0.38368900
H	0.63469500	3.65231000	1.50946600
H	1.88826600	1.52788500	1.85064900
H	-1.29298300	2.02747700	-1.98794800
H	0.62423000	-2.66570200	0.92964300
H	-1.09289900	-2.47698500	-1.12553000
H	-0.10580100	-0.62984000	-2.73114700
H	3.32934300	-2.06489800	0.21417100
H	3.69784100	-0.32786100	0.13585600
H	2.95718200	-1.01636300	1.59933500
H	-4.24546500	-0.27061300	0.30149000
H	-3.73699300	-1.36677300	-1.00078600
H	-3.26562600	0.34298800	-1.04902100

TSXS (ba)

C	3.97233200	-0.49578900	-0.32752100
C	3.76536700	0.87159900	-0.48632900
C	2.48646000	1.43516300	-0.30132600
C	1.45000600	0.59172200	0.04699600
C	1.66055500	-0.78856200	0.20828300
C	2.90762900	-1.35090800	0.02125100
C	-0.05493900	0.79634600	0.33795400
C	-0.81000100	0.13983700	-0.85254400
C	-0.56756600	-1.20122900	-0.71395200
C	0.26898800	-1.33452400	0.56210800
O	-0.24327500	-0.23273100	1.34028200
C	-3.09570900	0.21031800	-0.31699400
N	-3.20075900	-0.95263600	-0.01732800
O	-2.59940500	-2.02103800	0.08209900
C	-0.48535000	2.15181900	0.84865300
C	-3.88613700	1.44281500	-0.50515100

H	4.96708500	-0.90983600	-0.46978000
H	4.60010100	1.51499900	-0.75207600
H	2.33651400	2.50515200	-0.42525300
H	3.07680900	-2.41786800	0.14532500
H	-1.00172000	0.65022700	-1.79028800
H	-0.64581500	-1.96825200	-1.47209300
H	0.20782100	-2.27041700	1.11520800
H	-1.51564300	2.10950700	1.21173600
H	-0.42392200	2.90391500	0.05399600
H	0.15748600	2.46958600	1.67528700
H	-3.71172000	1.86135800	-1.50260300
H	-4.95594600	1.22997300	-0.40449400
H	-3.61411700	2.20863100	0.22872200

TSNS (ba)

C	-2.98722200	-0.78936100	0.04307700
C	-2.51050400	-0.71197800	1.35091100
C	-1.31356600	-0.03175400	1.64156300
C	-0.63322900	0.56308400	0.59345300
C	-1.12179400	0.49471500	-0.72062300
C	-2.28873300	-0.18419800	-1.01708500
C	0.65396700	1.39356300	0.48566200
C	1.69623600	0.55080800	-0.31775200
C	1.22187500	0.54480600	-1.60170100
C	-0.11497400	1.30780800	-1.53629500
O	0.22888000	2.32455700	-0.55813600
C	1.48883000	-1.64403600	0.26982900
N	1.00041700	-2.06205600	-0.75254400
O	0.62425500	-1.72424100	-1.87698300
C	1.14985100	2.12667300	1.70985100
C	1.90706100	-2.06080800	1.62111600
H	-3.91561700	-1.31659500	-0.15991100
H	-3.07367400	-1.17482200	2.15719100
H	-0.95470400	0.03392900	2.66655600
H	-2.66648100	-0.24851600	-2.03407700
H	2.73645800	0.47763500	-0.02001900
H	1.75206500	0.31526600	-2.51387500
H	-0.46726300	1.75739600	-2.46438100
H	2.01608800	2.74680400	1.45840600
H	0.36328500	2.77347100	2.11009700
H	1.44731600	1.41872300	2.49176900
H	1.93045200	-3.15326100	1.69621700
H	1.21081000	-1.67658700	2.37542900
H	2.90647200	-1.67751200	1.85332800

TSXA (bb)

C	-4.04868100	-2.44333200	0.01733700
C	-4.82055700	-1.28573200	0.06341800
C	-4.21982000	-0.01325300	-0.01787800
C	-2.84674500	0.04804900	-0.15317600

C	-2.06798300	-1.12112200	-0.19631500
C	-2.64682000	-2.37159500	-0.11095300
C	-1.82700700	1.20433800	-0.27255000
C	-1.05184300	1.18287200	1.05898500
C	-0.26230900	0.06642200	1.01758900
C	-0.62855300	-0.60332700	-0.32678100
O	-0.85134300	0.56309000	-1.14090700
O	0.56474200	2.89628100	0.63774100
N	1.49954000	2.11423300	0.49291000
C	1.82417900	0.94888300	0.50859400
H	-4.53169700	-3.41512700	0.07698000
H	-5.90054700	-1.36247300	0.15828400
H	-4.83084200	0.88548300	0.01562100
H	-2.05121200	-3.28078100	-0.14838000
H	-1.32379500	1.76774300	1.92725500
H	0.11297200	-0.46672500	1.88367100
H	0.10717400	-1.26562700	-0.78297200
C	2.93666400	0.08206600	0.20933100
C	3.98205900	0.52999800	-0.62423200
C	2.99049900	-1.22041900	0.73423100
C	5.05479000	-0.30794800	-0.90998200
H	3.93855400	1.53338900	-1.03546100
C	4.06616500	-2.05416900	0.43541600
H	2.19083500	-1.57153400	1.37792300
C	5.10141500	-1.60258700	-0.38455300
H	5.85635900	0.04976600	-1.55034400
H	4.09612500	-3.05857900	0.84843200
H	5.93932700	-2.25449500	-0.61466200
C	-2.29622000	2.52612300	-0.82959300
H	-3.02267400	2.98856600	-0.15170500
H	-1.44588000	3.20300700	-0.93953300
H	-2.77407200	2.38118400	-1.80347500

TSNA (bb)

C	0.84168500	2.94391800	-0.55600100
C	1.89946600	2.89922400	0.35162700
C	2.58713300	1.69833400	0.60070600
C	2.19045900	0.56838100	-0.09096100
C	1.12139100	0.61251200	-0.99877200
C	0.43261400	1.78705500	-1.24290500
C	2.69265100	-0.88282600	-0.14478000
C	1.60775000	-1.79263200	0.48240200
C	0.53695500	-1.74307000	-0.36845600
C	1.02360200	-0.81990100	-1.52224900
O	2.43189100	-1.16188100	-1.55835200
C	-1.02147900	-0.60823500	0.88025600
N	-0.33944400	-0.40787400	1.86409500
O	0.77424600	-0.59680700	2.34696300
C	4.12911200	-1.16345700	0.22725600
H	0.32926600	3.88478900	-0.73888600

H	2.20129200	3.80562700	0.86988400
H	3.40736600	1.67210500	1.31324000
H	-0.39658700	1.82689700	-1.94500600
H	1.80400700	-2.50606500	1.26996200
H	-0.21246300	-2.51538800	-0.49324500
H	0.56131500	-0.97056200	-2.49838200
H	4.37265100	-2.21488700	0.04465300
H	4.80464100	-0.54041000	-0.36641400
H	4.29538900	-0.94794800	1.28816600
C	-2.35934900	-0.37430100	0.39360900
C	-3.32768700	0.21041700	1.23608000
C	-2.71908100	-0.72674700	-0.91786500
C	-4.61755000	0.43450200	0.76743100
H	-3.05222500	0.48381200	2.24957400
C	-4.01515600	-0.49874300	-1.37667900
H	-1.98217100	-1.17807600	-1.57356900
C	-4.96840700	0.08156400	-0.53914600
H	-5.35354900	0.88691400	1.42642600
H	-4.27887200	-0.77629200	-2.39342900
H	-5.97769300	0.25813900	-0.89985600

TSXS (bb)

C	-5.12163700	-0.68532900	-0.26073400
C	-4.45869200	-1.90939400	-0.24302700
C	-3.06699300	-1.97433200	-0.02836300
C	-2.38490900	-0.78987900	0.16960500
C	-3.05556700	0.44476500	0.15245600
C	-4.41702200	0.51949600	-0.06556200
C	-0.90353900	-0.43167700	0.43407200
C	-0.40386300	0.27248000	-0.86004700
C	-1.09064000	1.45784000	-0.89358300
C	-1.93875700	1.47333300	0.38198000
O	-1.08994800	0.73052000	1.28103700
C	1.76187700	1.07477800	-0.35423100
N	1.43944500	2.23299500	-0.20417000
O	0.49321900	3.01363100	-0.24672200
C	-0.04804300	-1.48023100	1.10592600
H	-6.19591000	-0.65706200	-0.42298200
H	-5.02038900	-2.82789600	-0.39197600
H	-2.55934800	-2.93592600	-0.01344300
H	-4.94141600	1.47199500	-0.07960600
H	-0.04116300	-0.26284700	-1.73023800
H	-1.26922200	2.09167400	-1.75154000
H	-2.20749500	2.44146200	0.80162300
H	0.92027300	-1.06342600	1.39221300
H	0.12719700	-2.32523800	0.43070300
H	-0.54817000	-1.85434300	2.00455000
C	2.91022800	0.20874000	-0.23120200
C	3.92747200	0.50180200	0.69967600
C	3.02612800	-0.93918700	-1.03353500

C	5.03541000	-0.33303600	0.80855400
H	3.83629500	1.38507400	1.32375600
C	4.13627300	-1.77183700	-0.91212400
H	2.24579800	-1.16943800	-1.75156900
C	5.14410700	-1.47251600	0.00650800
H	5.81580500	-0.09482200	1.52604500
H	4.21542100	-2.65499800	-1.53988700
H	6.00903700	-2.12326400	0.09881100

TSNS (bb)

C	-2.09241100	2.82042300	-0.43313200
C	-1.00500600	2.57438200	-1.27115200
C	-0.57269100	1.25998200	-1.52473600
C	-1.26761900	0.22239200	-0.92825800
C	-2.36663200	0.47187000	-0.09190100
C	-2.78776600	1.76112900	0.17601200
C	-1.14382400	-1.30832100	-0.96293300
C	-0.71051100	-1.78508800	0.46039900
C	-1.80786000	-1.56737100	1.24917900
C	-2.84932500	-0.92038400	0.31469300
O	-2.56590300	-1.64683400	-0.90985000
C	0.79518500	-0.27317100	1.30428000
N	0.07789800	0.23502800	2.14207200
O	-1.05508400	0.18778100	2.61807800
C	-0.46387300	-1.95433500	-2.14678200
H	-2.41227500	3.84360700	-0.25410300
H	-0.48891100	3.40777200	-1.74098800
H	0.27751900	1.07702700	-2.17693400
H	-3.63252000	1.95940300	0.83045800
H	0.03969600	-2.55146400	0.61480300
H	-2.03265100	-1.98986500	2.21742300
H	-3.89494100	-1.02650000	0.60290200
H	-0.54062700	-3.04453100	-2.08192100
H	-0.93374000	-1.62799500	-3.07951000
H	0.59671000	-1.68163600	-2.17628400
C	2.08605300	-0.09428800	0.68318900
C	2.63854300	1.19599000	0.55466200
C	2.79862000	-1.19769100	0.18293600
C	3.88234200	1.36591400	-0.04559600
H	2.08143700	2.04883800	0.92817900
C	4.03873100	-1.01567600	-0.42591200
H	2.38050500	-2.19450500	0.27992600
C	4.58566300	0.26375000	-0.54014000
H	4.30201800	2.36428200	-0.13355900
H	4.58096900	-1.87677200	-0.80636900
H	5.55371100	0.40253100	-1.01319200

TSXA (ca)

C	-3.63162400	-2.22051300	0.08032700
C	-3.86518000	-0.93518400	0.55921200

C	-2.82943000	0.01989500	0.60309300
C	-1.57712000	-0.34939200	0.14828600
C	-1.34225900	-1.65554700	-0.31964300
C	-2.34859500	-2.59918500	-0.36296200
C	-0.20152700	0.36578900	0.04400600
C	0.63085400	-0.31896500	1.14935600
C	0.90578800	-1.58121200	0.69671300
C	0.15538200	-1.67087300	-0.65032000
O	0.32601900	-0.32983100	-1.13468000
O	2.90938600	0.62714600	1.07573100
N	3.36416000	-0.36913700	0.51044600
C	3.11130900	-1.46569900	0.08535800
C	3.68127500	-2.63268000	-0.61104900
H	-4.44478900	-2.94085500	0.04833300
H	-4.85969400	-0.65991200	0.90043300
H	-3.02828400	1.01845600	0.98356800
H	-2.16896100	-3.60802700	-0.72762100
H	0.69729000	0.04141000	2.16611600
H	1.11304700	-2.43904300	1.32758700
H	0.49982600	-2.40106100	-1.38416600
H	4.75968500	-2.50580300	-0.75455600
H	3.21585900	-2.76322500	-1.59466300
H	3.51461400	-3.54969900	-0.03511600
C	1.50093700	2.70987700	-1.07645900
H	1.56125500	3.78987600	-1.26055800
H	2.35188900	2.41038000	-0.45845600
H	1.58684000	2.19692600	-2.04075100
C	-0.28323400	3.11876800	1.44630900
H	-0.27958200	4.20946900	1.32981100
H	-1.21062100	2.84781300	1.96543800
H	0.55715700	2.85449300	2.09860900
C	-1.56239700	2.76816500	-1.36993600
H	-2.54390500	2.58738400	-0.91932200
H	-1.49864100	3.83547500	-1.61634100
H	-1.52354600	2.20795700	-2.31141800
Si	-0.12834900	2.26814000	-0.23944300

TSNA (ca)

C	-2.23590100	2.71966800	-0.10771800
C	-1.24811200	2.82897000	0.86907900
C	-0.18755200	1.90712100	0.93236400
C	-0.14268800	0.89120100	-0.00676500
C	-1.15302700	0.77185400	-0.97680600
C	-2.20012500	1.67304800	-1.04677300
C	0.84219800	-0.25552200	-0.31203900
C	0.12872400	-1.58728600	0.03196900
C	-0.89869500	-1.71219400	-0.86541500
C	-0.75580300	-0.46346100	-1.77912000
O	0.68225200	-0.29416800	-1.78203200
C	-2.72487800	-1.44167400	0.47316300

N	-2.16231900	-1.25636000	1.52561800
O	-1.04892400	-1.17611000	2.04980700
C	-4.06378200	-1.50197700	-0.14181700
H	-3.03760400	3.45243200	-0.14884700
H	-1.29088100	3.64272100	1.58826100
H	0.57058600	2.00366200	1.70443600
H	-2.96979200	1.59326400	-1.81184900
H	0.54132700	-2.35386500	0.67139900
H	-1.34386300	-2.64217400	-1.20008900
H	-1.14273200	-0.55368000	-2.79505500
H	-4.84005500	-1.52982500	0.63035600
H	-4.16517100	-2.39641000	-0.76592500
H	-4.23579000	-0.62372000	-0.77456100
Si	2.70621400	-0.09729600	0.10400800
C	3.58566900	-1.55894900	-0.71080600
H	4.67171800	-1.49399300	-0.57191400
H	3.25544300	-2.51646200	-0.29089800
H	3.38090600	-1.57972900	-1.78660600
C	2.94141800	-0.16401900	1.98220700
H	4.00939800	-0.17156400	2.23353400
H	2.49021100	0.69710400	2.48793900
H	2.49391900	-1.06728600	2.41308000
C	3.34173300	1.53343100	-0.60579700
H	2.84609500	2.39522400	-0.14507900
H	4.42146900	1.64127600	-0.44625000
H	3.15235400	1.58065800	-1.68391800

TSXS (ca)

C	-4.25124600	-0.79586600	0.35609100
C	-3.88395300	0.41396100	0.93729000
C	-2.55116500	0.86924000	0.87859200
C	-1.61874900	0.08856200	0.22074000
C	-1.99300900	-1.14052100	-0.35372800
C	-3.29417400	-1.59880100	-0.29540200
C	-0.09244800	0.20649000	-0.04445300
C	0.53714000	-0.87357100	0.89241100
C	0.13946900	-2.07070800	0.35320100
C	-0.67725900	-1.71734600	-0.89118800
O	-0.02110800	-0.50905600	-1.31620400
C	2.86613200	-1.09509200	0.59191100
N	2.82440500	-2.07873700	-0.10753500
O	2.06716500	-2.89446900	-0.63275000
C	3.82311300	-0.25548600	1.34165000
H	-5.28523700	-1.12680900	0.40603300
H	-4.63329800	1.01955500	1.44039200
H	-2.28141300	1.81442000	1.34343700
H	-3.58292300	-2.54942100	-0.73758500
H	0.72717100	-0.69964400	1.94558800
H	0.09433800	-3.02969000	0.85117300
H	-0.72270400	-2.44848300	-1.69714500
H	3.70539300	0.80339300	1.09414400

H	3.66794700	-0.36685000	2.42138600
H	4.85225600	-0.55223900	1.11139700
Si	0.65296000	1.95733800	-0.30839300
C	2.16849400	1.81917500	-1.42861000
H	1.86234000	1.44356100	-2.41100100
H	2.63546300	2.80150900	-1.57234600
H	2.92878800	1.13189500	-1.04746300
C	1.08774400	2.71468300	1.37652600
H	1.53073700	3.71023700	1.24962500
H	0.19721700	2.83304200	2.00603900
H	1.80513600	2.10409300	1.93699900
C	-0.61811200	3.04619700	-1.18954600
H	-1.49249800	3.26570600	-0.56859000
H	-0.16529800	4.00195300	-1.48163500
H	-0.97602000	2.55490300	-2.10147300

TSNS (ca)

C	2.74096600	-2.27309100	0.71157400
C	1.80937400	-2.06292400	1.72643500
C	0.63104400	-1.33367700	1.48314800
C	0.41550700	-0.84042700	0.20653800
C	1.35552200	-1.06216200	-0.81509300
C	2.52301100	-1.76356100	-0.58074300
C	-0.70969000	-0.03016600	-0.46156600
C	-0.11014000	1.37278200	-0.81950300
C	0.75893600	1.13175700	-1.85151700
C	0.74376800	-0.39472700	-2.04590400
O	-0.65912000	-0.66211000	-1.79736700
C	1.33887600	2.03874500	0.82641400
N	2.37490200	1.91857400	0.21639900
O	2.84074300	1.58971600	-0.87737400
C	0.80868200	2.42143800	2.14842900
H	3.64330000	-2.84243200	0.91827900
H	1.99024100	-2.47266700	2.71687300
H	-0.08815800	-1.18069700	2.28434700
H	3.25582800	-1.92360000	-1.36723800
H	-0.64164100	2.30278900	-0.65236100
H	1.15693000	1.83423800	-2.56862700
H	1.05054200	-0.76667000	-3.02366600
H	1.59948700	2.86341800	2.76402400
H	0.40830900	1.54646300	2.67206200
H	0.00062900	3.15395000	2.04643100
C	-3.59382100	0.79080800	-1.10767800
H	-3.42246600	0.40241600	-2.11727300
H	-4.66014800	0.67952800	-0.87631000
H	-3.36879200	1.86381700	-1.12228500
C	-2.70824700	0.66050200	1.85466100
H	-3.75851200	0.62975900	2.17050900
H	-2.12349200	0.14175600	2.62314000
H	-2.40181800	1.71342100	1.85241100
C	-3.01118100	-1.96116300	0.20907600

H	-2.40356200	-2.51508600	0.93355200
H	-4.06471700	-2.08352500	0.48822600
H	-2.86199300	-2.42726700	-0.77084500
Si	-2.52449400	-0.13823500	0.14330400

TSXA (da)

C	3.73183300	-1.61768600	0.01902800
C	3.92483400	-0.28926000	-0.35330400
C	2.84591300	0.61527000	-0.40041700
C	1.59837200	0.13894900	-0.04990900
C	1.39773500	-1.20135200	0.31862300
C	2.45011500	-2.09500000	0.35711600
C	0.18767000	0.76345600	0.02584800
C	-0.59389600	0.14761700	-1.14960900
C	-0.82344300	-1.15239600	-0.79171600
C	-0.11245300	-1.30075700	0.57475100
O	-0.36139500	0.00648900	1.13278200
O	-2.75345700	1.11620800	-0.71969400
N	-3.24721100	0.04894400	-0.35324500
C	-3.04212700	-1.12257600	-0.17350500
C	-3.65389400	-2.38641500	0.27379000
H	4.58000600	-2.29646300	0.05000500
H	4.92219900	0.05679900	-0.61115800
H	2.98816300	1.64909400	-0.69865800
H	2.30755800	-3.13437400	0.64334300
H	-0.65394300	0.60592500	-2.12618000
H	-0.98773800	-1.97404500	-1.47995900
H	-0.45736200	-2.08365700	1.25081400
H	-4.71061200	-2.23517400	0.51884300
H	-3.14546200	-2.77109400	1.16500100
H	-3.58607500	-3.15028100	-0.50869200
C	0.09847100	2.27029200	0.19007700
O	0.66508100	2.97278900	-0.62781600
C	-0.70663200	2.80639400	1.34505300
H	-0.61625100	3.89381600	1.38097400
H	-1.75429200	2.51666400	1.20465800
H	-0.37254600	2.35707900	2.28658900

TSNA (da)

C	-1.42877100	2.85299900	-0.11006200
C	-0.47449100	2.85748400	0.90738400
C	0.47921300	1.82935200	1.00961400
C	0.44229100	0.82687200	0.05953800
C	-0.52694700	0.80570300	-0.95422500
C	-1.47062100	1.81286700	-1.05617800
C	1.29953600	-0.42379000	-0.21403800
C	0.45500100	-1.67341900	0.11575800
C	-0.52963500	-1.70051200	-0.83719000
C	-0.22180700	-0.47023600	-1.73901800
O	1.22867600	-0.44716700	-1.67003000

C	-2.40038900	-1.25013200	0.36072400
N	-1.88472300	-1.10684300	1.44386800
O	-0.80338600	-1.12530300	2.03149500
C	-3.70334100	-1.19945000	-0.32841100
H	-2.14752500	3.66552200	-0.17593000
H	-0.46293700	3.66984000	1.62895300
H	1.21584500	1.82417300	1.80750900
H	-2.21612300	1.81846600	-1.84844100
H	0.78513100	-2.45129800	0.78683600
H	-1.03867300	-2.58507800	-1.20128400
H	-0.55977700	-0.52327900	-2.77402800
H	-4.52066600	-1.15841300	0.39941600
H	-3.84531400	-2.08566500	-0.95637500
H	-3.76685300	-0.31348300	-0.97072800
C	2.72290500	-0.38312700	0.31394600
O	2.92534900	-0.59942500	1.49365000
C	3.81295100	-0.03397300	-0.67159800
H	3.60086000	0.93405100	-1.14034400
H	4.77566700	-0.00541900	-0.15784900
H	3.83294600	-0.77018500	-1.48320200

TSXS (da)

C	4.08734600	-0.56489400	-0.27487400
C	3.78063400	0.73372400	-0.67321500
C	2.45876600	1.21780800	-0.60568500
C	1.48960400	0.36341600	-0.12108000
C	1.79262600	-0.94955400	0.27840200
C	3.08453400	-1.43232300	0.20275600
C	-0.03835500	0.47758800	0.10282800
C	-0.70690400	-0.41048200	-0.97544100
C	-0.38012500	-1.68608400	-0.59830800
C	0.43638100	-1.54119800	0.69181000
O	-0.17862500	-0.36440900	1.26615300
C	-2.95974800	-0.32963900	-0.46631500
N	-3.02632300	-1.41824100	0.04855200
O	-2.38514300	-2.42751000	0.34163700
C	-3.77310800	0.82363000	-0.90252500
H	5.11404700	-0.91628700	-0.33251400
H	4.56962200	1.38471900	-1.03999700
H	2.21756300	2.22792000	-0.92582200
H	3.33261700	-2.44657600	0.50569800
H	-0.90259900	-0.05890500	-1.98040200
H	-0.39517400	-2.57833700	-1.20870300
H	0.42720400	-2.37060000	1.39684200
H	-4.15894400	0.66699400	-1.91721900
H	-4.62298000	0.97367100	-0.22723700
H	-3.16658600	1.73259000	-0.91114000
C	-0.55924000	1.88359100	0.31846900
O	-0.78685700	2.59033900	-0.64955200
C	-0.73221800	2.34669800	1.74447300

H	0.21566400	2.25264900	2.28713600
H	-1.07614800	3.38275100	1.75755900
H	-1.44618800	1.69606600	2.26224500

TSNS (da)

C	2.45157000	-2.01369600	0.97885400
C	1.55892300	-1.67423400	1.99584200
C	0.33389000	-1.05019000	1.70155500
C	0.04655400	-0.80087400	0.37189200
C	0.93771500	-1.14690900	-0.65389600
C	2.15118100	-1.74539100	-0.36782300
C	-1.14999500	-0.17779500	-0.37165400
C	-0.69101300	1.18073500	-0.98783900
C	0.15125500	0.81307700	-2.00337000
C	0.22330600	-0.72494100	-1.93814400
O	-1.15218900	-1.02144900	-1.55628200
C	0.68133400	2.17555600	0.48459700
N	1.72164100	2.02883000	-0.11018900
O	2.20838800	1.56027800	-1.14435200
C	0.06980100	2.71291300	1.71431000
H	3.39174000	-2.49739700	1.22980600
H	1.81003900	-1.89910800	3.02899600
H	-0.36103400	-0.78150600	2.49238500
H	2.85495800	-2.00741200	-1.15318900
H	-1.30776400	2.06967300	-0.94181800
H	0.48424900	1.40321400	-2.84374800
H	0.49136100	-1.24237400	-2.85857500
H	0.75773900	2.61681000	2.56139000
H	-0.84451600	2.15290300	1.93339500
H	-0.19505800	3.77047000	1.59449100
C	-2.46573300	-0.17408100	0.37575400
O	-2.61301000	0.59461700	1.31299300
C	-3.52515600	-1.15059600	-0.06680300
H	-3.13339100	-2.17315900	-0.01375900
H	-4.41091600	-1.04747100	0.56263800
H	-3.77620000	-0.97545800	-1.11921300

3X (aa)

C	-3.50047800	1.05946400	-0.40504600
C	-3.70473100	-0.32102900	-0.44391600
C	-2.66721800	-1.21237600	-0.12614800
C	-1.44564400	-0.67957600	0.25315800
C	-1.24035700	0.70945800	0.29063500
C	-2.25193400	1.59375600	-0.04721400
C	-0.09572600	-1.27108000	0.62226900
C	0.83719900	-1.06965500	-0.60962700
C	1.08844000	0.46139500	-0.56186400
C	0.21977700	0.86397200	0.68612000
O	0.41623600	-0.27764200	1.53560600
O	2.12668300	-1.68003800	-0.40926500

N	3.10325400	-0.68926000	-0.21303800
C	2.57531300	0.47447200	-0.30765200
C	3.40643900	1.70961100	-0.16064200
H	-4.31948900	1.73011200	-0.65047200
H	-4.68071200	-0.71136400	-0.71927400
H	-2.83164200	-2.28618300	-0.16641700
H	-2.09895900	2.66999000	-0.02724100
H	-0.06007800	-2.26272800	1.07147700
H	0.41636000	-1.46166400	-1.53884300
H	0.80784900	1.02019500	-1.45992000
H	0.51609100	1.77927300	1.19917700
H	4.45366200	1.44203000	-0.00138700
H	3.06947000	2.31649100	0.68975800
H	3.33483000	2.33963600	-1.05674900

3N (aa)

C	2.71870400	1.33699300	-0.14205800
C	2.94966800	0.39774200	0.86533900
C	2.10500700	-0.71105400	1.02494600
C	1.05047000	-0.85650000	0.13868100
C	0.81176600	0.09229100	-0.86737400
C	1.63129800	1.20025400	-1.01837000
C	-0.05520800	-1.87918700	-0.02932800
C	-1.40501200	-1.26508900	0.47606800
C	-1.68223900	-0.18897800	-0.59934300
C	-0.44357000	-0.39907300	-1.56011400
O	-0.29107000	-1.83159000	-1.45556900
O	-1.32659600	-0.56326700	1.72786800
N	-1.50398900	0.81732300	1.50820800
C	-1.72353300	1.04386000	0.26377700
C	-1.97460500	2.43453000	-0.22706000
H	3.39169700	2.18312500	-0.25135500
H	3.79797400	0.52525700	1.53221500
H	2.28408500	-1.43239000	1.81753800
H	1.45446700	1.93844200	-1.79696900
H	0.14519100	-2.90166600	0.28965600
H	-2.17448100	-2.03656900	0.56228900
H	-2.60649800	-0.34358600	-1.16532100
H	-0.60214100	-0.10864500	-2.59854000
H	-1.97960100	3.13626800	0.61033100
H	-2.93874000	2.49687900	-0.74797900
H	-1.19918200	2.74573900	-0.93869400

3X (ab)

C	-4.04475400	2.07236800	-0.28453800
C	-4.77169500	0.88490500	-0.38865600
C	-4.16510100	-0.35590600	-0.13511100
C	-2.83313200	-0.36209300	0.24664600
C	-2.10152800	0.83251700	0.34910900
C	-2.68737100	2.05783100	0.07513400

C	-1.82365400	-1.45190500	0.56623900
C	-0.88122200	-1.57298400	-0.66743000
C	-0.05896900	-0.26233800	-0.56587100
C	-0.69728600	0.38393400	0.72179600
O	-0.96384600	-0.78559700	1.51234600
O	0.07435300	-2.64132800	-0.49738400
N	1.34926000	-2.11837300	-0.29438800
C	1.32389600	-0.83125600	-0.34760100
H	-4.53682900	3.02132100	-0.47983300
H	-5.82207200	0.92140800	-0.66445000
H	-4.73551600	-1.27690800	-0.22502100
H	-2.12702000	2.98676600	0.14694000
H	-2.18164200	-2.39876300	0.96868100
H	-1.41146500	-1.74093600	-1.60781800
H	-0.11979400	0.39501400	-1.43709100
H	-0.06076900	1.07842100	1.26921500
C	2.55227800	-0.03955800	-0.18774900
C	2.53461100	1.35325800	-0.36490400
C	3.77141500	-0.66278000	0.14005800
C	3.70170700	2.10474200	-0.22164100
H	1.60713400	1.85659400	-0.62269900
C	4.93159300	0.08954600	0.28236400
H	3.78842400	-1.73832800	0.28055200
C	4.90343800	1.47690200	0.10275300
H	3.66856500	3.18148100	-0.36459700
H	5.86438800	-0.40646100	0.53697100
H	5.81235600	2.06130400	0.21658200

3N (ab)

C	1.50337000	2.89281900	-0.27266100
C	2.55963000	2.58963100	0.58967700
C	3.02422100	1.27314800	0.72574900
C	2.42076600	0.29047700	-0.04220200
C	1.35771600	0.59443300	-0.90584900
C	0.87571700	1.88864400	-1.02484900
C	2.61224000	-1.20566300	-0.18449400
C	1.43075300	-1.94432000	0.53303700
C	0.23734300	-1.60792500	-0.38994300
C	0.95754200	-0.74144300	-1.49942700
O	2.22729600	-1.42717200	-1.56006200
O	1.08589900	-1.42439900	1.82991900
N	-0.16605200	-0.80497500	1.77325800
C	-0.67210300	-0.91078500	0.59057900
H	1.16274100	3.92076100	-0.36249800
H	3.02903400	3.38497500	1.16222900
H	3.83603400	1.04093600	1.40965500
H	0.04217000	2.12764200	-1.67986000
H	3.60485000	-1.61356200	0.00451700
H	1.64264200	-3.01102300	0.63931400
H	-0.22348500	-2.48390800	-0.85533600

H	0.47975300	-0.74219100	-2.47875800
C	-2.00236000	-0.36632500	0.28393200
C	-2.55442800	-0.51575000	-0.99833900
C	-2.74980900	0.31015400	1.26664600
C	-3.81857500	-0.00388200	-1.29387600
H	-1.99873900	-1.04033200	-1.77060700
C	-4.00837300	0.81886200	0.96813400
H	-2.32568300	0.42800300	2.25823500
C	-4.54958100	0.66517200	-0.31316300
H	-4.23019400	-0.13084600	-2.29157500
H	-4.57282500	1.33903700	1.73747400
H	-5.53390500	1.06440300	-0.54214800

3X (ba)

C	3.48731100	-1.34292800	-0.27200600
C	3.69596900	0.00741200	-0.55848500
C	2.66238400	0.94520500	-0.40224700
C	1.43930700	0.49516200	0.06955500
C	1.23101100	-0.86294000	0.35459400
C	2.23782300	-1.79834200	0.17883700
C	0.09712100	1.17025000	0.33972500
C	-0.83490900	0.73280400	-0.84566400
C	-1.09325400	-0.76178300	-0.52477800
C	-0.22706300	-0.93820100	0.77399200
O	-0.41803000	0.33243500	1.40913900
O	-2.12711400	1.36888400	-0.78244600
N	-3.10669900	0.43551900	-0.40106200
C	-2.57977800	-0.72546600	-0.27399600
C	-3.41172700	-1.90978400	0.10478600
H	4.30310500	-2.05013800	-0.39530000
H	4.67221400	0.33821200	-0.90256100
H	2.83187900	1.99358600	-0.63445900
H	2.08031800	-2.85260000	0.39322500
H	-0.40348500	0.95011100	-1.82602700
H	-0.81652600	-1.47502200	-1.30756000
H	-0.52434400	-1.74992300	1.43912900
H	-4.45845800	-1.61600500	0.21296000
H	-3.07227000	-2.34511800	1.05352300
H	-3.34221900	-2.69755900	-0.65652400
C	0.07042200	2.63102100	0.71973200
H	0.66598500	2.79792600	1.62202000
H	0.48292400	3.24359200	-0.08966000
H	-0.95877000	2.94928100	0.90085500

3N (ba)

C	2.39598600	-2.01695000	0.05929400
C	2.79010300	-1.05761100	-0.87575800
C	2.14184300	0.18443800	-0.95134000
C	1.11514000	0.43884500	-0.05617200
C	0.71328200	-0.52896900	0.87540100

C	1.33611400	-1.76566500	0.94367900
C	0.20096500	1.63247500	0.18457900
C	-1.22907500	1.26858600	-0.35841200
C	-1.69404300	0.17381900	0.62556700
C	-0.45200600	0.10922100	1.60210300
O	-0.06627000	1.49764200	1.60913300
O	-1.25110000	0.66562600	-1.66322600
N	-1.65246400	-0.68109000	-1.55482100
C	-1.92131700	-0.96578900	-0.33201300
C	-2.39931100	-2.33211000	0.04563700
H	2.91837900	-2.96873400	0.10480700
H	3.61251700	-1.27456600	-1.55197700
H	2.44801200	0.92121400	-1.68894500
H	1.03069900	-2.51856700	1.66640200
H	-1.86101300	2.16141600	-0.38504600
H	-2.59056300	0.43196400	1.19867600
H	-0.67092400	-0.23125200	2.61428600
H	-2.50998300	-2.95392000	-0.84594800
H	-3.36564800	-2.27900200	0.56343000
H	-1.69102600	-2.82133000	0.72645100
C	0.71335700	3.01188200	-0.15491600
H	-0.00002500	3.77493600	0.17334800
H	1.67444500	3.19884800	0.33321200
H	0.84511100	3.10745600	-1.23809500

4X (ba)

C	3.75770700	-0.46423200	-0.48944300
C	3.51076200	0.89559600	-0.68659100
C	2.25108300	1.44785400	-0.40257500
C	1.27113300	0.60781200	0.10206000
C	1.52039400	-0.75829000	0.30116400
C	2.75254100	-1.31508300	-0.00217400
C	-0.19115100	0.80990000	0.50250900
C	-1.04141300	0.15802400	-0.67121500
C	-0.75296900	-1.35028400	-0.44276600
C	0.19413500	-1.31252900	0.78877600
O	-0.33885000	-0.19824400	1.52541100
C	-2.54296300	0.16354600	-0.50035700
N	-3.03760100	-0.97681700	-0.18410100
O	-2.02408400	-1.94239900	-0.10989600
C	-0.59148200	2.17042800	1.02758900
C	-3.45178500	1.32898300	-0.74854500
H	4.74128000	-0.86890200	-0.71218000
H	4.30466100	1.53636400	-1.06083800
H	2.06615100	2.50668300	-0.56646200
H	2.94889900	-2.37462200	0.14155300
H	-0.73852200	0.55171700	-1.64646500
H	-0.33512900	-1.89508700	-1.29400300
H	0.19451800	-2.21589000	1.39779200
H	-1.59202200	2.13327300	1.46618600

H	-0.58551400	2.91807000	0.22686000
H	0.10975700	2.49030700	1.80426500
H	-3.33011100	1.69915200	-1.77522900
H	-4.49154200	1.02285100	-0.61000900
H	-3.24168400	2.16859500	-0.07748500

4N (ba)

C	-3.11043000	-0.67220200	0.42405600
C	-2.75022300	0.33923000	1.31688200
C	-1.55820800	1.05973700	1.14515200
C	-0.76502700	0.75403300	0.04962700
C	-1.13280000	-0.25611600	-0.85089700
C	-2.29324700	-0.99096300	-0.67083100
C	0.57268900	1.27338600	-0.46041700
C	1.66385300	0.14827900	-0.19502300
C	1.25610200	-0.92928800	-1.22290900
C	-0.01401700	-0.28308100	-1.87100200
O	0.40471500	1.09718100	-1.89293400
C	1.58530000	-0.65632200	1.07584300
N	1.21177100	-1.87235700	0.90165100
O	1.01470700	-2.12925100	-0.46942300
C	0.97446800	2.69315200	-0.13402100
C	1.88939400	-0.14443200	2.44861800
H	-4.03745800	-1.21786900	0.57748000
H	-3.40210000	0.57320900	2.15425300
H	-1.28272400	1.84121300	1.84919900
H	-2.57276000	-1.78663700	-1.35601800
H	2.65765400	0.57900100	-0.36025900
H	2.01107400	-1.14757500	-1.98280600
H	-0.25345600	-0.62651800	-2.87725700
H	0.19614700	3.39199500	-0.45485500
H	1.12751400	2.81575900	0.94385700
H	1.90740900	2.95238400	-0.64487800
H	2.90812800	0.26109000	2.49817400
H	1.79344700	-0.94950700	3.18103000
H	1.20223400	0.66402500	2.72892400

3X (bb)

C	-3.76265700	2.48462700	-0.21581300
C	-4.55576200	1.35540700	-0.42749700
C	-4.02742000	0.06396500	-0.26919500
C	-2.70506400	-0.05513000	0.12849900
C	-1.90834300	1.08106100	0.33761400
C	-2.41520200	2.35805000	0.15882100
C	-1.77996900	-1.24310100	0.38025200
C	-0.82151600	-1.29685700	-0.86091900
C	0.07537600	-0.05357700	-0.64164100
C	-0.54081500	0.52040800	0.68801900
O	-0.88539000	-0.68723100	1.37846900
O	0.07215700	-2.42964000	-0.79793900

N	1.37197700	-2.00434700	-0.52789500
C	1.41937500	-0.71875400	-0.45959900
H	-4.19422700	3.47431100	-0.33877400
H	-5.59690600	1.47698800	-0.71397200
H	-4.65067200	-0.80967300	-0.44266400
H	-1.80166100	3.24199600	0.31503100
H	-1.35523900	-1.34806300	-1.81295700
H	0.06790400	0.67723800	-1.45474000
H	0.12713300	1.13212600	1.29411300
C	2.68701300	-0.01735600	-0.20883700
C	2.75584400	1.38342900	-0.27775400
C	3.85756100	-0.73619500	0.09936500
C	3.96019500	2.04979300	-0.04808300
H	1.86749800	1.96001200	-0.51946700
C	5.05516500	-0.06848300	0.32810200
H	3.80757200	-1.81837500	0.15649600
C	5.11327500	1.32760500	0.25617300
H	3.99421900	3.13431100	-0.10797200
H	5.94954900	-0.63787500	0.56653000
H	6.05094900	1.84574900	0.43765200
C	-2.37343300	-2.55417500	0.83696400
H	-2.92871100	-2.41231300	1.76874000
H	-3.05844300	-2.94914800	0.07850900
H	-1.57865700	-3.28617800	0.99766300

3N (bb)

C	1.00157000	3.09667700	-0.28683600
C	2.08497400	2.88876100	0.56990900
C	2.66480000	1.61843700	0.70336300
C	2.14733900	0.58425900	-0.06045900
C	1.05731300	0.79331400	-0.91656900
C	0.46183500	2.03955100	-1.03440300
C	2.49020500	-0.89195400	-0.20142600
C	1.36334900	-1.72126500	0.51819000
C	0.14022300	-1.49689500	-0.39430600
C	0.77429600	-0.57183700	-1.50816700
O	2.09626100	-1.14123000	-1.57950500
O	0.98269500	-1.22913800	1.81708800
N	-0.32026700	-0.72576400	1.76868700
C	-0.82329000	-0.88244400	0.59027900
H	0.57065000	4.09029800	-0.37545600
H	2.48486400	3.72268000	1.14042800
H	3.49811300	1.46121700	1.38275700
H	-0.39226700	2.20265700	-1.68631400
H	1.66996900	-2.76528300	0.62955300
H	-0.24201700	-2.41184300	-0.85615500
H	0.28898400	-0.61339500	-2.48314500
C	-2.19930900	-0.46244200	0.29014800
C	-2.75143900	-0.69239900	-0.98000300
C	-2.99112200	0.17119100	1.26660200

C	-4.05961900	-0.30211000	-1.26977800
H	-2.16097400	-1.18609700	-1.74667900
C	-4.29337000	0.55926100	0.97364100
H	-2.56686200	0.35191900	2.24855100
C	-4.83475100	0.32509600	-0.29532700
H	-4.47055800	-0.49070900	-2.25793000
H	-4.89208700	1.04802500	1.73764700
H	-5.85319300	0.63031400	-0.51960400
C	3.91155000	-1.33212000	0.05678700
H	4.03235900	-2.39323000	-0.18491400
H	4.61140300	-0.75311200	-0.55293300
H	4.16452100	-1.18862700	1.11285200

4X (bb)

C	4.05500800	-1.99919900	-0.46679700
C	4.77651700	-0.81287800	-0.61261100
C	4.18505900	0.42846900	-0.32840700
C	2.87589200	0.43552900	0.12560000
C	2.14937700	-0.75566200	0.27061900
C	2.71951800	-1.98191800	-0.03281600
C	1.88430300	1.52479200	0.49157900
C	0.88263800	1.63692000	-0.68951700
C	0.07281000	0.32096300	-0.55399600
C	0.75729200	-0.32258100	0.73267000
O	1.07553900	0.87046400	1.48269600
O	-0.06651600	2.70030300	-0.45861200
N	-1.34107800	2.17403000	-0.27689400
C	-1.31532600	0.88723200	-0.34927400
H	4.53412400	-2.94915300	-0.68806900
H	5.80997000	-0.85069300	-0.94622100
H	4.74976200	1.34928700	-0.45103800
H	2.16386500	-2.91065800	0.07094500
H	2.26352100	2.47562400	0.86474500
H	1.36083700	1.81295400	-1.65669600
H	0.13638500	-0.34538200	-1.41784300
C	-2.56787800	0.11677400	-0.26431500
C	-2.63213300	-1.20994200	-0.71992900
C	-3.73630900	0.70976700	0.24976200
C	-3.82864600	-1.92518800	-0.66513700
H	-1.74661900	-1.68603300	-1.13084700
C	-4.92701600	-0.00700200	0.30387500
H	-3.69110900	1.73430400	0.60361000
C	-4.97981700	-1.32808800	-0.15211000
H	-3.85894600	-2.94978000	-1.02608300
H	-5.81890400	0.46501800	0.70728400
H	-5.91108100	-1.88595300	-0.10564800
C	-0.03521500	-1.29055800	1.58145200
H	-0.96418500	-0.83305600	1.92984900
H	-0.28862200	-2.19280700	1.01566800
H	0.55992700	-1.58259000	2.45204400

4N (bb)

C	1.50849200	2.73595200	-1.04214900
C	2.55047200	2.73128700	-0.11202100
C	3.00774400	1.53050100	0.45027400
C	2.41205000	0.35106700	0.03342700
C	1.36368800	0.35434700	-0.89722600
C	0.88935600	1.54043800	-1.43685900
C	2.59952000	-1.10837400	0.38922400
C	1.40490200	-1.56872700	1.28877300
C	0.22830600	-1.55640100	0.28796600
C	0.96166800	-1.10633100	-1.05229000
O	2.23982000	-1.76649900	-0.84092500
O	1.04770700	-0.64581900	2.33463200
N	-0.20306600	-0.08679800	2.06257300
C	-0.69496700	-0.57944000	0.97553700
H	1.17230200	3.67830700	-1.46625500
H	3.01382600	3.67012400	0.17895400
H	3.80900400	1.53307800	1.18427800
H	0.06859800	1.55483700	-2.14903100
H	3.58679000	-1.42871000	0.72171900
H	1.60784200	-2.54008300	1.74669200
H	-0.22332500	-2.54038100	0.12828300
C	-2.02570400	-0.16002300	0.50649600
C	-2.72030300	-0.91353200	-0.45327600
C	-2.63520500	0.99707800	1.02667800
C	-3.98963100	-0.52348700	-0.88274900
H	-2.27673100	-1.81877100	-0.85662300
C	-3.90019200	1.38228800	0.59623100
H	-2.09912000	1.58329700	1.76542600
C	-4.58345500	0.62548600	-0.36150000
H	-4.51372400	-1.12188700	-1.62315400
H	-4.35573300	2.28007000	1.00553000
H	-5.57039300	0.93149000	-0.69766700
C	0.34444900	-1.54806100	-2.35888100
H	1.01565800	-1.30773900	-3.18887300
H	0.17068600	-2.62941800	-2.35611000
H	-0.61155400	-1.04248500	-2.52675500

3X (ca)

C	-3.48633900	-2.19725100	0.08508800
C	-3.68854600	-0.94026800	0.65628700
C	-2.65775200	0.01300700	0.68589000
C	-1.43988800	-0.31419500	0.10692900
C	-1.23823600	-1.58654900	-0.45554300
C	-2.24194000	-2.54128900	-0.46664400
C	-0.09601300	0.40714300	-0.02431500
C	0.81341500	-0.27919100	1.05371700
C	1.07535700	-1.67796400	0.43310000
C	0.21880500	-1.58575800	-0.87891700

O	0.42066900	-0.21598600	-1.24543900
O	2.11532100	0.33772800	1.16324100
N	3.09681200	-0.49685900	0.59803800
C	2.56474700	-1.59693700	0.21246000
C	3.39725600	-2.67523900	-0.40580200
H	-4.29982500	-2.91748300	0.06690900
H	-4.65795000	-0.69308800	1.08068100
H	-2.82660900	0.98289900	1.14633700
H	-2.08329000	-3.52825800	-0.89462100
H	0.36400400	-0.27417900	2.04927400
H	0.79013200	-2.53400200	1.05280900
H	0.51564400	-2.25115600	-1.69100500
H	4.44789700	-2.37609500	-0.42631600
H	3.07430100	-2.88398300	-1.43387400
H	3.30677500	-3.61217600	0.15888700
Si	-0.01038900	2.32484000	-0.21289100
C	1.62248400	2.78093300	-1.03524700
H	1.68626900	3.86295800	-1.20499200
H	2.46974800	2.47368500	-0.41581600
H	1.71698600	2.27919500	-2.00428100
C	-0.15079800	3.09759700	1.51030300
H	0.67885600	2.77691500	2.15045600
H	-0.11446600	4.19192100	1.44374900
H	-1.08868600	2.83215200	2.01310000
C	-1.45201500	2.87191800	-1.31012500
H	-2.42881500	2.65132600	-0.86605200
H	-1.40507400	3.95245000	-1.49415500
H	-1.40928000	2.36749700	-2.28237600

3N (ca)

C	-2.25676400	2.83324600	-0.03311100
C	-1.21120200	2.95915400	0.88265800
C	-0.17105800	2.01823800	0.92524100
C	-0.19261900	0.96988700	0.01673600
C	-1.25695800	0.83761600	-0.89031500
C	-2.29760700	1.75230300	-0.92658400
C	0.72970400	-0.21467900	-0.25773100
C	0.01549400	-1.50554600	0.30175600
C	-1.19453100	-1.66387400	-0.64788300
C	-0.96785900	-0.44883700	-1.63004700
O	0.47214000	-0.43609600	-1.68507500
O	-0.53307400	-1.37160400	1.62438200
N	-1.94019400	-1.40766900	1.55906100
C	-2.32244500	-1.58914400	0.34674100
C	-3.77715500	-1.69155300	0.01273600
H	-3.04685200	3.57897300	-0.05433800
H	-1.19993500	3.79923400	1.57186000
H	0.62623500	2.12077000	1.65562200
H	-3.12044400	1.64945900	-1.63018000
H	0.69431900	-2.36252000	0.30515700

H	-1.19646700	-2.59623900	-1.22214600
H	-1.38797800	-0.57017100	-2.62907400
H	-4.37929300	-1.63785600	0.92285500
H	-3.99441900	-2.63648800	-0.50172600
H	-4.08338600	-0.87788100	-0.65707000
C	3.42992900	-1.59526100	-0.73663400
H	4.52319300	-1.51805800	-0.69372800
H	3.14725300	-2.51516900	-0.21116400
H	3.14063500	-1.70675400	-1.78731700
C	2.96097800	0.00089300	1.88431200
H	2.43653700	-0.80172000	2.41562500
H	4.03394800	-0.11138300	2.08335700
H	2.64339600	0.95047800	2.32999500
C	3.24392300	1.49728800	-0.84211800
H	2.77195900	2.39927800	-0.43679300
H	4.32931800	1.60592500	-0.72725000
H	3.02061100	1.45950800	-1.91421000
Si	2.62280100	-0.06232000	0.02272100

4X (ca)

C	-4.13500700	-0.23143400	0.38729300
C	-3.56652400	0.83930300	1.07834300
C	-2.18686100	1.09193300	1.00853700
C	-1.40483100	0.26831700	0.21111400
C	-1.98050700	-0.81426100	-0.47392000
C	-3.33644800	-1.08676400	-0.38795800
C	0.10064600	0.19243400	-0.08965200
C	0.59699300	-1.03978000	0.79524400
C	-0.04381600	-2.23399200	0.02809100
C	-0.80496200	-1.52035700	-1.11834300
O	0.07936700	-0.42627000	-1.40865500
C	2.05167300	-1.44415400	0.71852500
N	2.26918500	-2.49372600	0.01346500
O	1.06163600	-3.00540500	-0.48067900
C	3.18198000	-0.81622500	1.47617700
H	-5.20559900	-0.40596100	0.45115200
H	-4.19923300	1.48925300	1.67691300
H	-1.75846700	1.92067900	1.56629500
H	-3.77887100	-1.93252300	-0.90849600
H	0.26612600	-0.92834200	1.83210400
H	-0.68014500	-2.89525700	0.62362700
H	-0.97715300	-2.12780200	-2.00660800
H	3.32466800	0.23788900	1.22054800
H	2.98769200	-0.86279600	2.55622000
H	4.10987100	-1.35491100	1.26825900
C	2.59523500	1.59858300	-1.32270700
H	3.31226400	0.90959000	-0.86744000
H	2.32391300	1.18593300	-2.30031700
H	3.10786600	2.55394900	-1.49097000
C	1.41641200	2.62844800	1.39928500

H	1.95805400	3.57402100	1.27152200
H	0.50040900	2.85463200	1.95825000
H	2.03454800	1.97960100	2.02886700
C	-0.11105100	3.02545100	-1.26035200
H	0.40879400	3.95944200	-1.50740700
H	-0.42298300	2.55715200	-2.20051800
H	-1.01695600	3.28281400	-0.70173100
Si	1.03252100	1.86907800	-0.29627900

4N (ca)

C	-2.89970900	2.30549000	0.36589400
C	-1.90199700	2.40585200	1.33657300
C	-0.70461500	1.68360100	1.21656300
C	-0.52561000	0.88679400	0.09378800
C	-1.53253600	0.79223700	-0.88137800
C	-2.72820600	1.47958600	-0.75480700
C	0.58609100	-0.04712600	-0.37670600
C	0.04690500	-1.53984700	-0.19567000
C	-1.02867300	-1.62406900	-1.30583700
C	-0.99040800	-0.18098000	-1.90349400
O	0.42756500	0.06819500	-1.83168700
C	-0.79767500	-1.87236600	1.00802700
N	-2.03549700	-2.08178100	0.73808000
O	-2.25640600	-1.97696000	-0.64859100
C	-0.31124900	-1.96945300	2.41965600
H	-3.81922200	2.87318000	0.47922800
H	-2.05242200	3.05262500	2.19684200
H	0.05684900	1.76135100	1.98818400
H	-3.51435200	1.38884600	-1.49952900
H	0.87194900	-2.24704300	-0.33015100
H	-0.82739800	-2.36950900	-2.07984200
H	-1.34479900	-0.08871600	-2.93049200
H	0.49879700	-2.70559400	2.50435600
H	-1.12955200	-2.26979900	3.07847200
H	0.08434700	-1.00805600	2.76832200
Si	2.43196700	0.34294400	-0.00855800
C	3.47221300	-0.87678300	-1.01121500
H	4.53696900	-0.62059200	-0.95204800
H	3.36420100	-1.90740800	-0.65240800
H	3.17795800	-0.85632500	-2.06604000
C	2.82233200	0.15048500	1.83589000
H	3.88456400	0.36331500	2.01092100
H	2.24726200	0.84327000	2.46102400
H	2.63150400	-0.86597900	2.19861600
C	2.76832200	2.11452500	-0.56702100
H	3.82491800	2.37652700	-0.43345600
H	2.51960400	2.23651900	-1.62674300
H	2.16935900	2.83708400	-0.00135600

3X (da)

C	3.54607200	-1.65383600	-0.03632200
C	3.73302200	-0.35587800	-0.51746700
C	2.67952700	0.57158500	-0.52926800
C	1.45816100	0.16229200	-0.01718600
C	1.26609400	-1.14239200	0.46043100
C	2.29606000	-2.06970500	0.44830000
C	0.09331800	0.82669200	0.12355200
C	-0.80178800	0.21761300	-1.01919200
C	-1.02795700	-1.22543200	-0.50056200
C	-0.20295200	-1.19784000	0.83878800
O	-0.44626000	0.14817800	1.28082400
O	-2.10912300	0.82244600	-1.05543100
N	-3.07648000	-0.08517600	-0.58245200
C	-2.52241500	-1.20483900	-0.29904300
C	-3.33232700	-2.35864400	0.20171800
H	4.37915300	-2.35152900	-0.03620800
H	4.71001900	-0.05798800	-0.88818600
H	2.81250100	1.57702000	-0.91360100
H	2.15399000	-3.08475600	0.81080600
H	-0.34765600	0.32693500	-2.00541500
H	-0.70147400	-2.02778300	-1.16876500
H	-0.50981800	-1.91195400	1.60352100
H	-4.38916900	-2.08570200	0.24712200
H	-3.00780100	-2.66539700	1.20434600
H	-3.21993700	-3.22996200	-0.45614400
C	0.03234500	2.34382000	0.22514400
O	0.70948100	3.00617500	-0.53998800
C	-0.90658300	2.93595500	1.24263100
H	-0.82381600	4.02438000	1.22829900
H	-1.93034300	2.62899400	0.99781800
H	-0.68652500	2.54322700	2.24119900

3N (da)

C	1.80093000	2.81398900	0.22553600
C	0.78112500	3.01152200	-0.70877600
C	-0.26961000	2.09192000	-0.84004000
C	-0.27284200	0.99699900	0.00911800
C	0.75705800	0.78620100	0.93655000
C	1.80834400	1.68295700	1.05520500
C	-1.20328900	-0.19072200	0.18927100
C	-0.50393600	-1.46632300	-0.44307800
C	0.65996300	-1.70383300	0.54598600
C	0.42321400	-0.53918200	1.58774600
O	-1.02045400	-0.50727300	1.59125100
O	0.09658000	-1.26306000	-1.72499200
N	1.50032500	-1.33256700	-1.60691300
C	1.83033700	-1.59631900	-0.39495900
C	3.26729900	-1.74955500	-0.00875000
H	2.59975000	3.54570300	0.31085300
H	0.80112500	3.89269700	-1.34413600

H	-1.05817900	2.22981400	-1.57127400
H	2.61001300	1.53016500	1.77371600
H	-1.21548800	-2.29290200	-0.52298400
H	0.61681100	-2.66625200	1.06585900
H	0.79994400	-0.72694400	2.59311100
H	3.90690000	-1.65493900	-0.88936900
H	3.44501300	-2.72777500	0.45600000
H	3.56128600	-0.98344900	0.71997900
C	-2.66645800	-0.02144100	-0.18348900
O	-2.95766200	0.50740700	-1.23961100
C	-3.69551300	-0.55692800	0.78543000
H	-3.50983200	-1.61554900	1.00273700
H	-3.61299400	-0.02812500	1.74189100
H	-4.69406300	-0.42677900	0.36432600

4X (da)

C	3.92576700	-0.47996300	-0.34016600
C	3.55759800	0.76875500	-0.84638700
C	2.23718800	1.23289200	-0.73605000
C	1.32617000	0.42064300	-0.08142500
C	1.68937400	-0.83498500	0.42587300
C	2.98522300	-1.30876000	0.29179100
C	-0.17102100	0.53628800	0.21623200
C	-0.89816600	-0.42191600	-0.81911100
C	-0.47215100	-1.80764200	-0.26499800
C	0.39619900	-1.41495700	0.96670900
O	-0.28556300	-0.22947600	1.42715700
C	-2.39774400	-0.52756100	-0.66728000
N	-2.79151300	-1.62483100	-0.13298500
O	-1.69282100	-2.45446000	0.14034700
C	-3.39230200	0.49524600	-1.12296900
H	4.95480300	-0.81524600	-0.43655600
H	4.30387500	1.39133600	-1.33222900
H	1.94187800	2.19527200	-1.14298800
H	3.27589200	-2.28526300	0.67050800
H	-0.59376700	-0.19388200	-1.84299900
H	0.04845500	-2.46586100	-0.96540300
H	0.44118300	-2.16405200	1.75611500
H	-3.28226800	0.68458500	-2.19826100
H	-4.40676700	0.13930800	-0.92853000
H	-3.25034200	1.45791600	-0.62026700
C	-0.70265800	1.95223800	0.34502800
O	-0.70720000	2.66626500	-0.64298500
C	-1.17507300	2.40278900	1.70469500
H	-1.52119500	3.43662000	1.65012300
H	-1.97672500	1.74553200	2.06150100
H	-0.36017700	2.31051800	2.43208600

4N (da)

C	2.94762300	-1.66519200	0.52381000
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C	1.99458600	-1.92997500	1.51038400
C	0.65929700	-1.53116000	1.34981500
C	0.31901300	-0.89308100	0.16761300
C	1.27079800	-0.63111300	-0.82708100
C	2.59674100	-0.99601100	-0.65782000
C	-0.97659900	-0.29933800	-0.37672600
C	-0.86670700	1.28699700	-0.31743300
C	0.17708700	1.54602300	-1.42628900
C	0.50595300	0.09321600	-1.91356800
O	-0.80789900	-0.50201500	-1.79835400
C	-0.17352300	1.91672500	0.86179600
N	0.98542900	2.39412700	0.58416900
O	1.26669100	2.22928800	-0.79072700
C	-0.73759200	2.00852300	2.24369600
H	3.97596100	-1.98226500	0.67368300
H	2.29098900	-2.45238900	2.41579600
H	-0.08044900	-1.72334000	2.12119900
H	3.34568000	-0.77876400	-1.41431300
H	-1.85348900	1.71940900	-0.51036800
H	-0.18251200	2.16121000	-2.25554400
H	0.87109600	0.01109800	-2.93684000
H	-1.63756800	2.63764600	2.24754000
H	-0.00226300	2.44273500	2.92499000
H	-1.04279600	1.02047700	2.60217100
C	-2.26277700	-0.89411200	0.16350000
O	-2.55568800	-0.69816000	1.33079700
C	-3.10514800	-1.72274000	-0.77437800
H	-3.99578200	-2.07659600	-0.25189000
H	-3.38433300	-1.13258900	-1.65474300
H	-2.51988700	-2.57100300	-1.14850800

Cartesian coordinates for TSXA (da) and TSXS (da) at M05-2X/ 6-311++g(2d,2p) level

TSXA (da)

C	3.68654100	-1.57596300	0.02793400
C	3.86871400	-0.25230500	-0.32830100
C	2.78844700	0.63847000	-0.37530200
C	1.55401900	0.14646200	-0.04273000
C	1.36345600	-1.18937200	0.31205800
C	2.41522000	-2.06771900	0.35189300
C	0.14466200	0.75015800	0.01146800
C	-0.60467000	0.13899500	-1.17325100
C	-0.82671500	-1.15537900	-0.82754900
C	-0.14239700	-1.30695500	0.54693600
O	-0.41184900	-0.00821600	1.10071000
O	-2.64758700	1.11224500	-0.67674200
N	-3.15079000	0.05808800	-0.31378900
C	-2.97794000	-1.09950600	-0.15883400

C	-3.50738400	-2.39678100	0.27758400
H	4.53544500	-2.23949500	0.05851400
H	4.85733800	0.10040400	-0.57301200
H	2.92075300	1.66857500	-0.66277900
H	2.28245400	-3.10210100	0.62705900
H	-0.65002000	0.60295700	-2.13910100
H	-0.99103500	-1.96849700	-1.51296600
H	-0.48235500	-2.09333100	1.20521200
H	-4.55803000	-2.29591900	0.53027600
H	-2.96577100	-2.74673600	1.15094300
H	-3.40065600	-3.12847400	-0.51683400
C	0.05113100	2.24223600	0.17171200
O	0.54263100	2.93393800	-0.68681600
C	-0.63602400	2.77064900	1.38822600
H	-0.59818100	3.85244300	1.38032300
H	-1.66342900	2.41504000	1.38244700
H	-0.15891200	2.36683600	2.27817300

TSXS (da)

C	4.05321600	-0.47552400	-0.21194600
C	3.72708400	0.81392500	-0.58870200
C	2.40112700	1.26490500	-0.53917800
C	1.45333700	0.38251700	-0.09419100
C	1.77558700	-0.92146600	0.28670100
C	3.06944700	-1.37091900	0.22919900
C	-0.07066600	0.45233100	0.08327400
C	-0.68407400	-0.42769200	-1.02060700
C	-0.33967600	-1.69221000	-0.65922700
C	0.43135900	-1.55317000	0.65382600
O	-0.22832600	-0.40362700	1.22167400
C	-2.86762500	-0.34998900	-0.44536700
N	-2.90895100	-1.43402500	0.02669000
O	-2.27524000	-2.45103900	0.26366700
C	-3.60091800	0.87714400	-0.79495600
H	5.08088700	-0.79747800	-0.25646100
H	4.50301800	1.48224700	-0.92461000
H	2.14104700	2.26635500	-0.84353600
H	3.33380200	-2.37591800	0.51720100
H	-0.88032300	-0.06540900	-2.01343900
H	-0.31862000	-2.56815400	-1.27827100
H	0.42177800	-2.39015700	1.33373000
H	-4.63071000	0.63005200	-1.03269800
H	-3.57966100	1.58459500	0.02830500
H	-3.13194500	1.34707600	-1.65204300
C	-0.62964000	1.82976000	0.28840500
O	-0.80017200	2.54349000	-0.67213300
C	-0.91928100	2.24489300	1.69625600
H	-0.01511600	2.14030200	2.29231400
H	-1.27891200	3.26591200	1.70921800
H	-1.64835000	1.56112300	2.12687300