Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information

Unraveling the Computed Non-least Motion Pathway for the Homodimerization of Superchameleonic Isocyanides: the Peculiar Nonsymmetrical $(F\text{-}NC)_2$ Reactant Complex

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1. Computational Methods

In our previous papers leading with the homodimerization of isocyanides[1,2] we used the DLPNO-CSSD(T)/ma-def2-TZVPP//wB97X-D/def2-TZVPD theoretical level. Nevertheless, we decided to reduce the theoretical level here used due to the big amount of data to analyse along the internal reaction coordinate and the computational cost that it requires. In any case, this supposed substantial differences in our results.

The geometries of the transition structures were fully optimized by using the wB97X-D hybrid functional[3] in combination with the def2-SVPD basis set.[4] The nature of transition structure was confirmed by performing a frequency analysis at the same level of theory. The stability of the wave functions was checked for all the optimized structures.[5] The resulting transition structure was submitted to a mass-weigthed Internal Reaction Coordinate calculation with the following specifications: SCF=(MaxCycle=1300, conver=12) Integral(UltraFine) irc(calcall, tight, maxcycle=1300, stepsize= –5, maxpoints=20000, forward/reverse). All calculations were performed by using the Gaussian 09.[6] All the analysed parameters were computed at each point of the IRC calculation and then they were collected to plot the corresponding graphs.

Initial search of conformational space of reactant complexes was done by using the semiempirical quantum mechanical methods GFN2-xTB, following the MTD-GC workflow, and the crest utility program implemented in the xTB program, which was recently developed by S. Grimme.[7] Next, the resulting geometries were fully optimized at the wB97X-D/def2-SVPD theoretical level.

Natural Orbital Bond analysis[8] were performed at wB97XD/def2-SVPD level with the NBO 7.0 software[9] and the NBO-orbitals were printed with the Jmol-NBO Visualization Helper.[10–12] The topological analysis of the electron density of the systems, the ellipticity parameter, was carried out within the framework of the Atoms in Molecules (AIM) methodology[13,14] by means of the AIMPAC package.[15]

2. Homodimerization of Me-NC vs F-NC

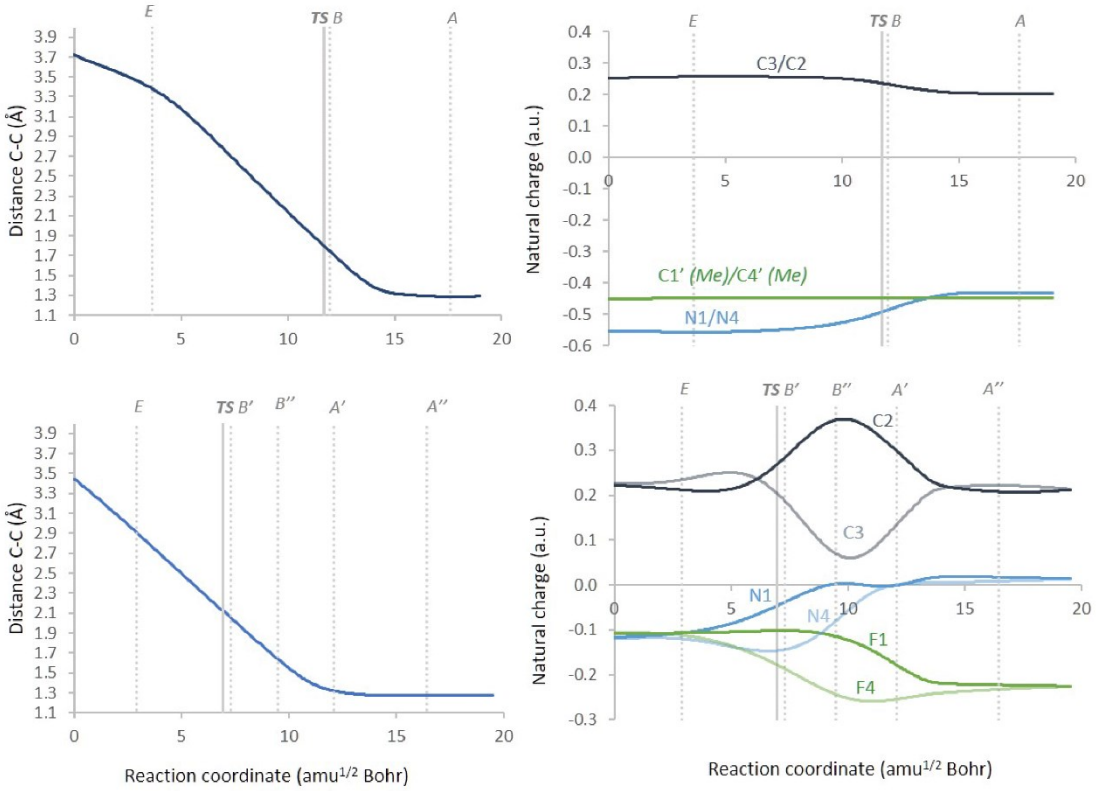


Figure S1. Computed evolution of the C2-C3 distance (Å, left) and of the natural charges at the individual atoms/group (a.u., right) along the reaction coordinate of the homodimerization of Me-NC (top) and F-NC (bottom) at the wB97X-D/def2-SVPD theoretical level.

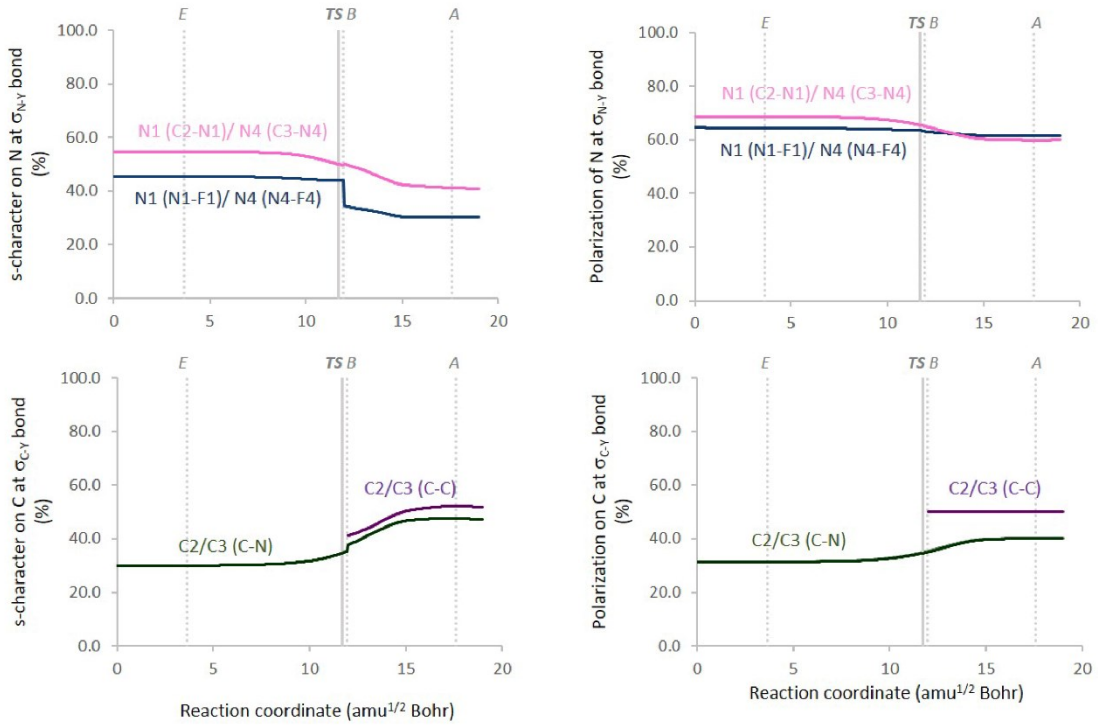


Figure S2. Computed evolution of the s-character on N/C at σ-$_{N/C-Y}$ bond (%, left) and of the polarization on N/C at σ-$_{N/C-Y}$ bond (%, right) along the reaction coordinate of the homodimerization of Me-NC at the wB97X-D/def2-SVPD theoretical level.

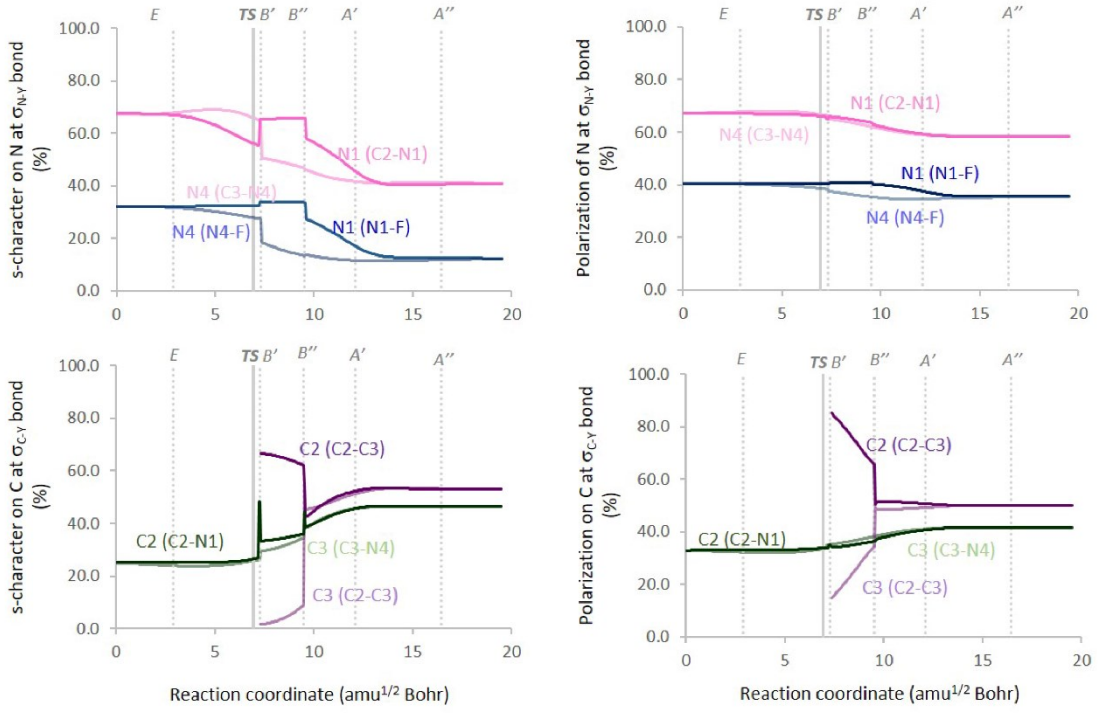


Figure S3. Computed evolution of the s-character on N/C at σ-$_{N/C-Y}$ bond (%, left) and of the polarization on N/C at σ-$_{N/C-Y}$ bond (%, right) along the reaction coordinate of the homodimerization of F-NC at the wB97X-D/def2-SVPD theoretical level.

3. Homodimerization of MeO-NC

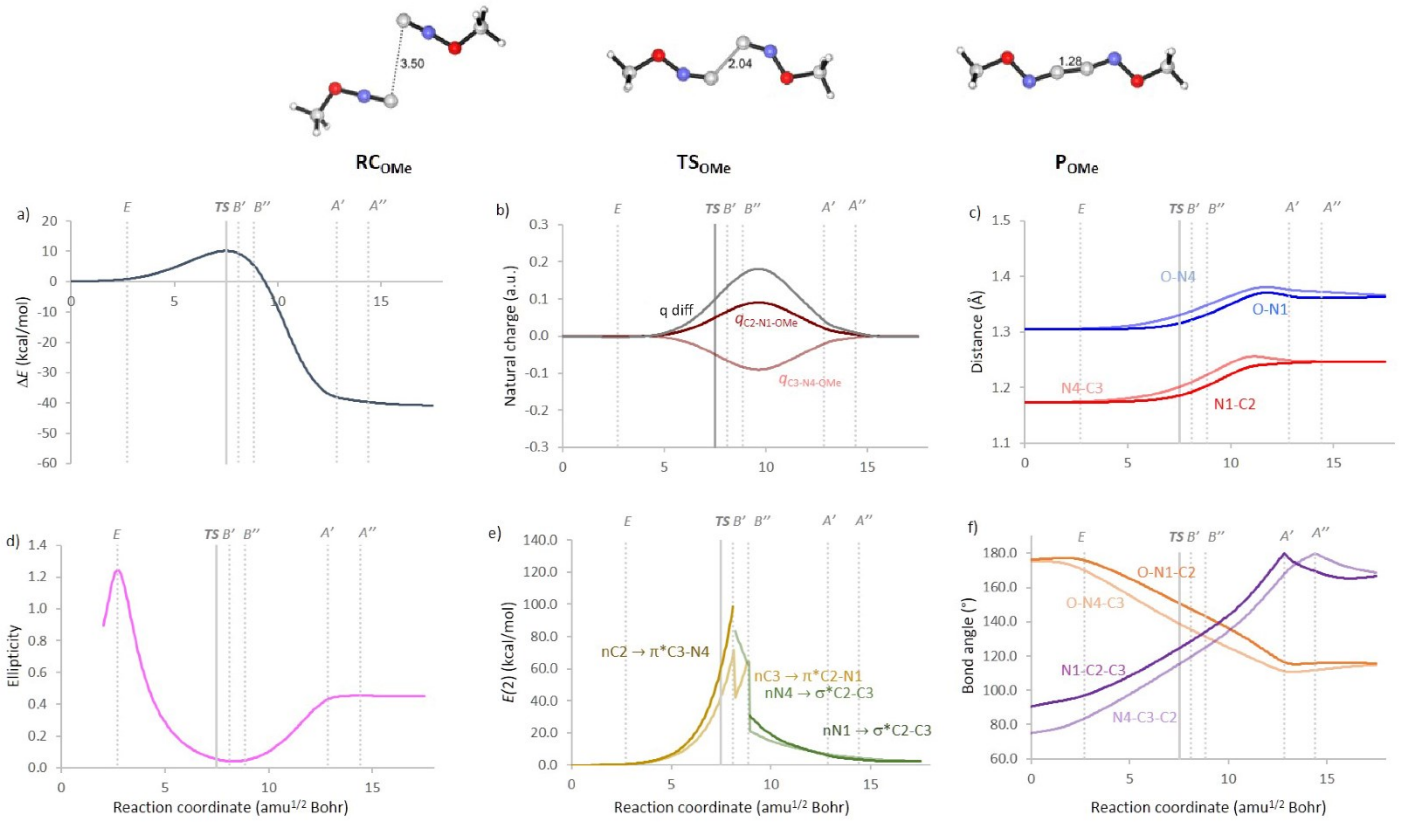


Figure S4. Computed potential energy profile (a), evolution of the total NBO-charges of the two monomers (b), the representative distances (Å,c), the ellipticity at the BCP of the C2-C3 bond (d), stabilizing orbital charge transfer interaction E(2) values (kcal mol^{-1},e) and the representative bond angles (°,f) along the reaction coordinate of the dimerization of MeO-NC (conformation of $\mathbf{TS_{OMe}}$) at the wB97X-D/def2-SVPD theoretical level. Numeration: left unit: MeO-N1-C2; right unit: C3-N4-OMe

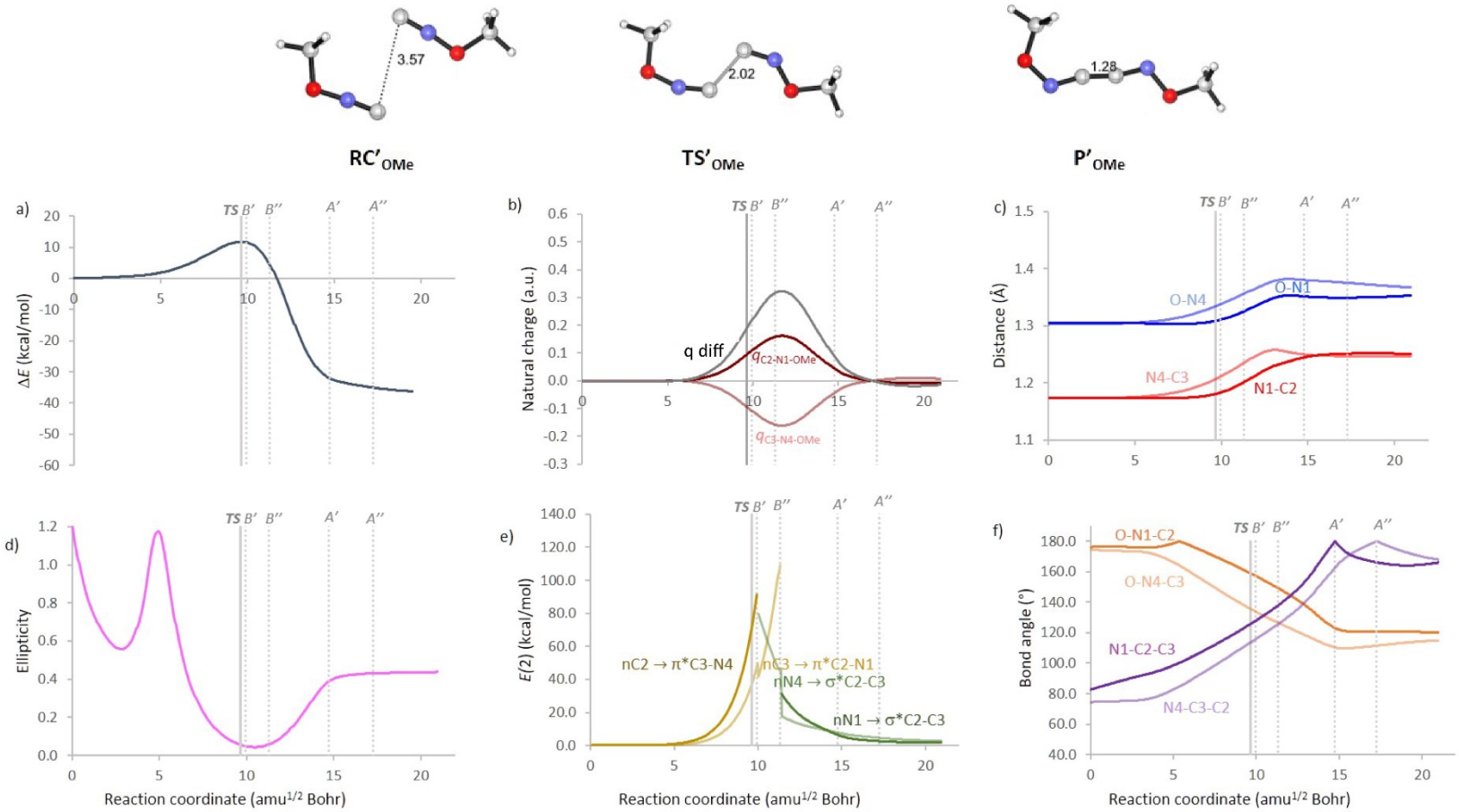


Figure S5. Computed potential energy profile (a), evolution of the total NBO-charges of the two monomers (b), the representative distances (Å,c), the ellipticity at the BCP of the C2-C3 bond (d), stabilizing orbital charge transfer interaction E(2) values (kcal mol^{-1},e) and the representative bond angles (°,f) along the reaction coordinate of the dimerization of MeO-NC (conformation of **TS'$_{OMe}$**) at the wB97X-D/def2-SVPD theoretical level. Numeration: left unit: MeO-N1-C2; right unit: C3-N4-OMe

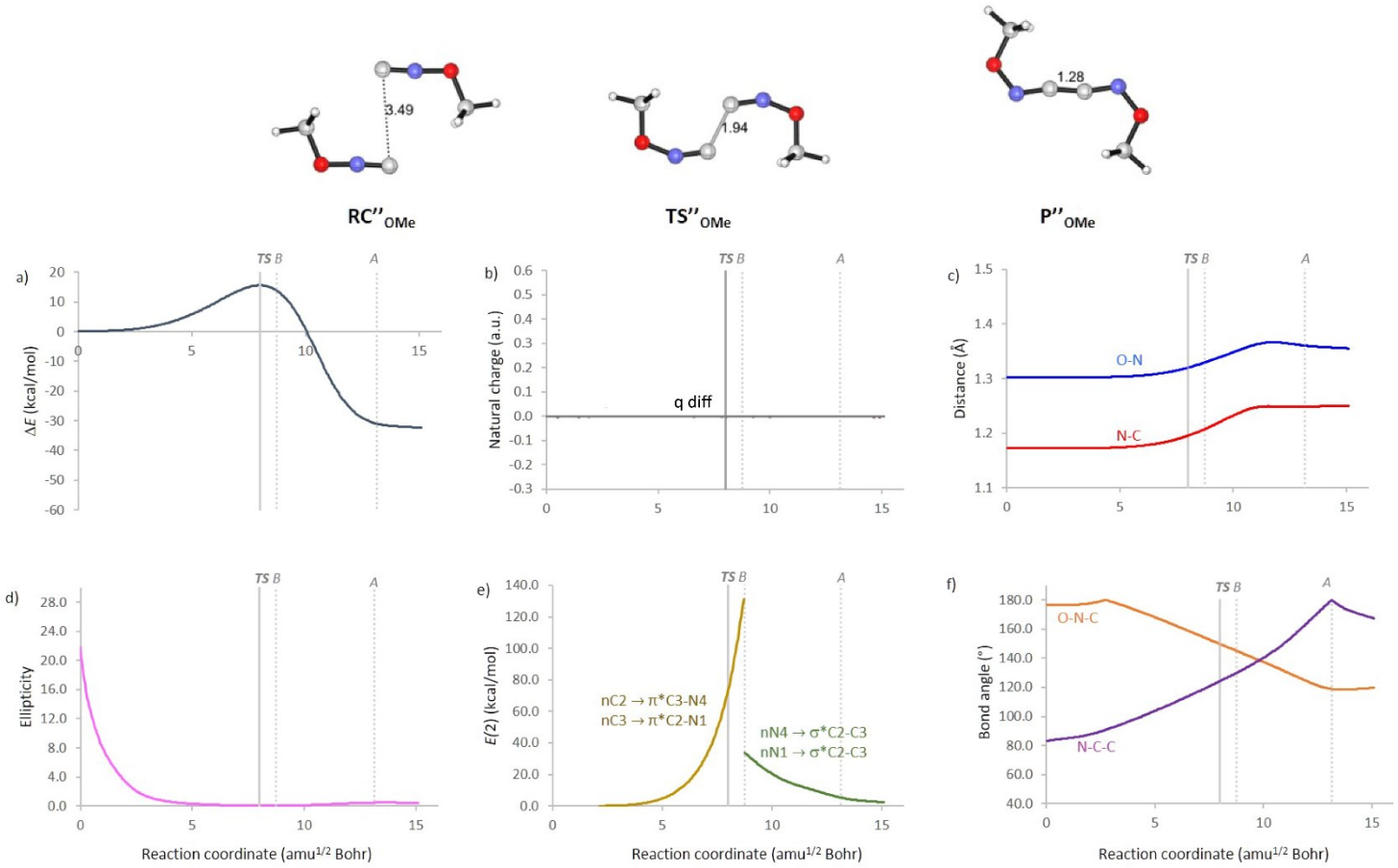
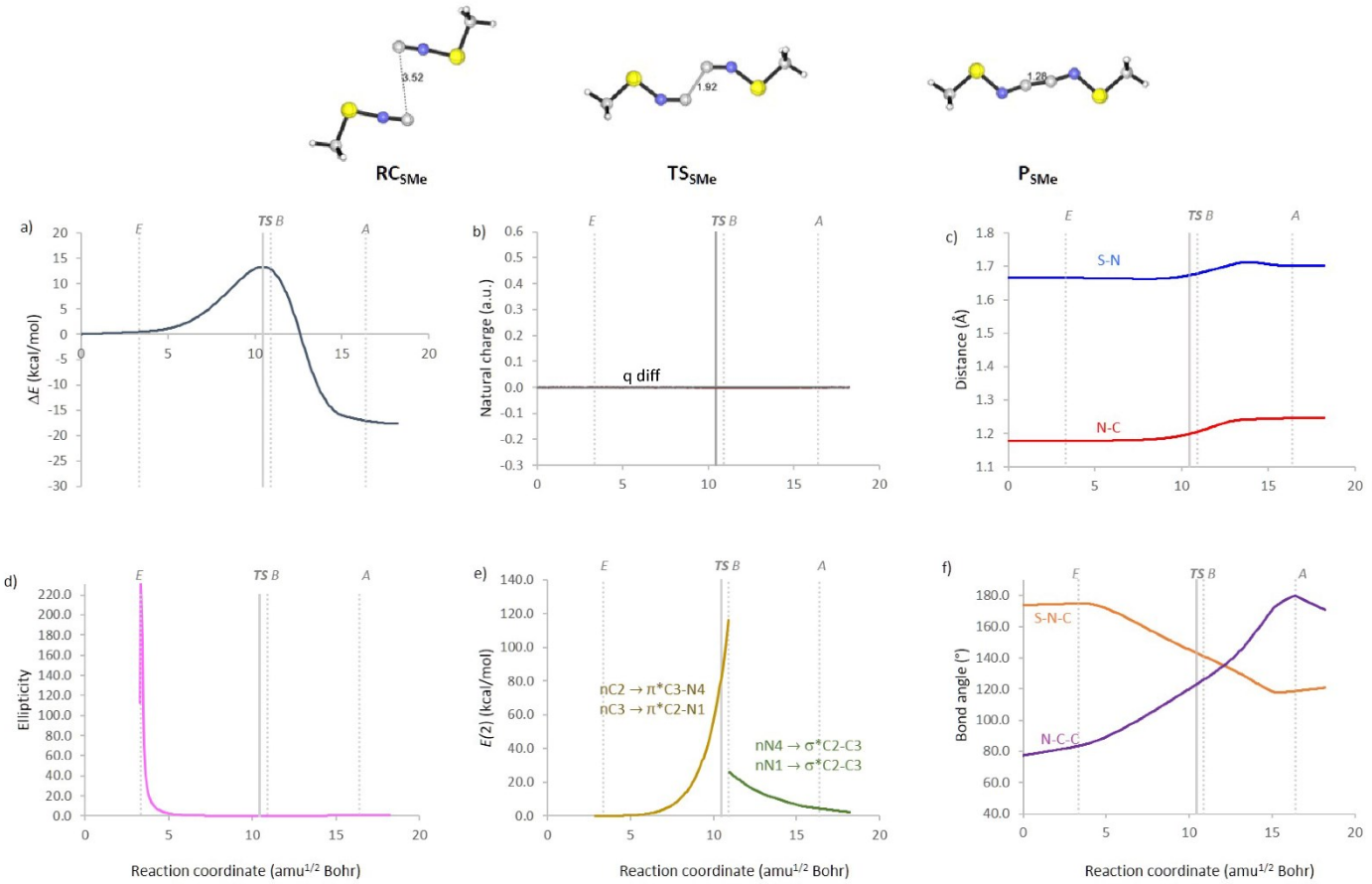


Figure S6. Computed potential energy profile (a), evolution of the total NBO-charges of the two monomers (b), the representative distances (Å,c), the ellipticity at the BCP of the C2-C3 bond (d), stabilizing orbital charge transfer interaction E(2) values (kcal mol^{-1},e) and the representative bond angles (°,f) along the reaction coordinate of the dimerization of MeO-NC (conformation of **TS''$_{OMe}$**) at the wB97X-D/def2-SVPD theoretical level. Numeration: left unit: MeO-N1-C2; right unit: C3-N4-OMe



4. Homodimerization of MeS-NC

Figure S7. Computed potential energy profile (a), evolution of the total NBO-charges of the two monomers (b), the representative distances (Å,c), the ellipticity at the BCP of the C2-C3 bond (d), stabilizing orbital charge transfer interaction E(2) values (kcal mol^{-1},e) and the representative

bond angles (°,f) along the reaction coordinate of the dimerization of MeS-NC (conformation of $\mathbf{TS_{SMe}}$) at the wB97X-D/def2-SVPD theoretical level. Numeration: left unit: MeS-N1-C2; right unit: C3-N4-SMe

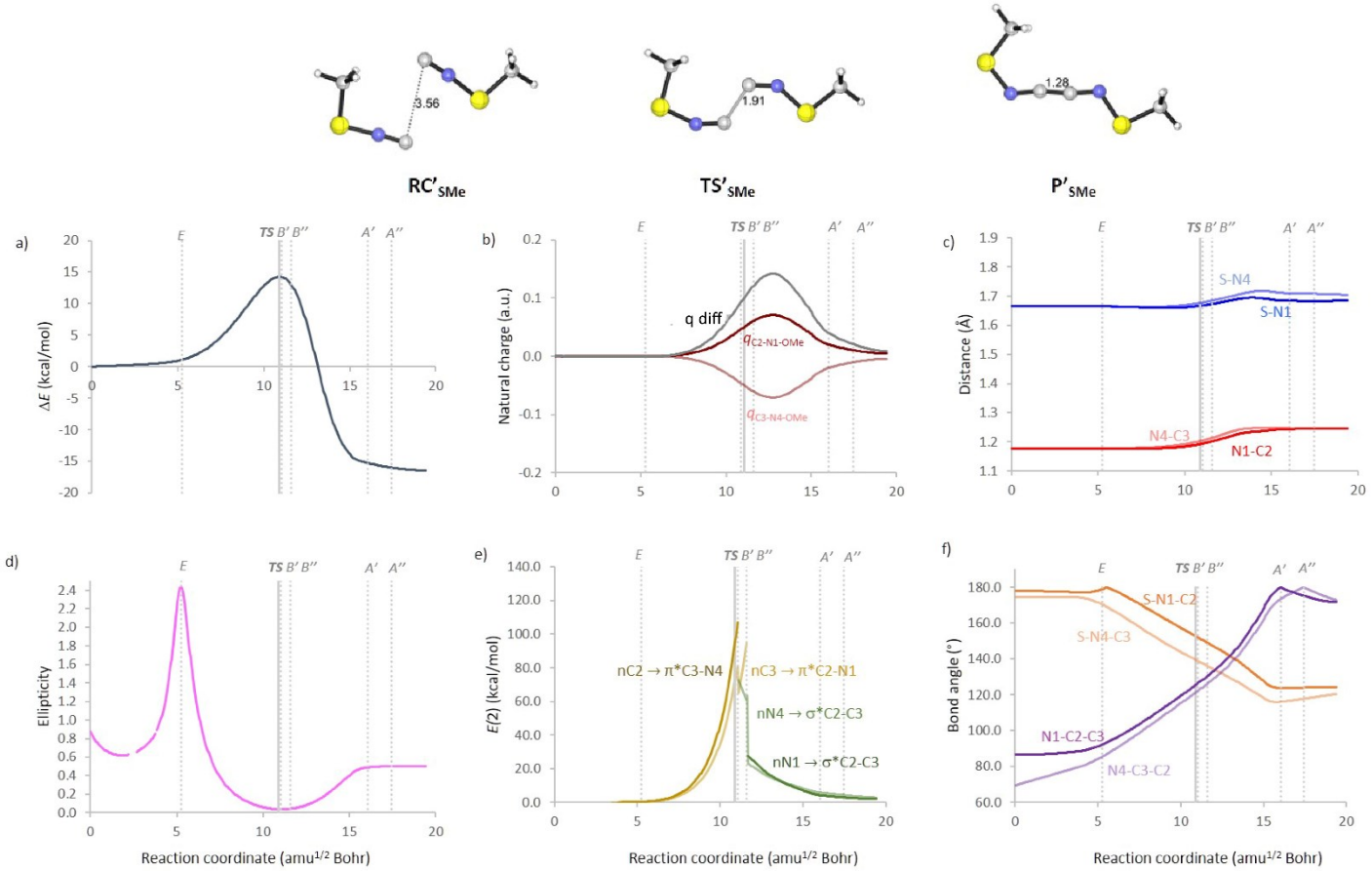


Figure S8. Computed potential energy profile (a), evolution of the total NBO-charges of the two monomers (b), the representative distances (Å,c), the ellipticity at the BCP of the C2-C3 bond (d), stabilizing orbital charge transfer interaction E(2) values (kcal mol^{-1},e) and the representative

bond angles (°,f) along the reaction coordinate of the dimerization of MeS-NC (conformation of **TS'$_{SMe}$**) at the wB97X-D/def2-SVPD theoretical level. Numeration: left unit: MeS-N1-C2; right unit: C3-N4-SMe

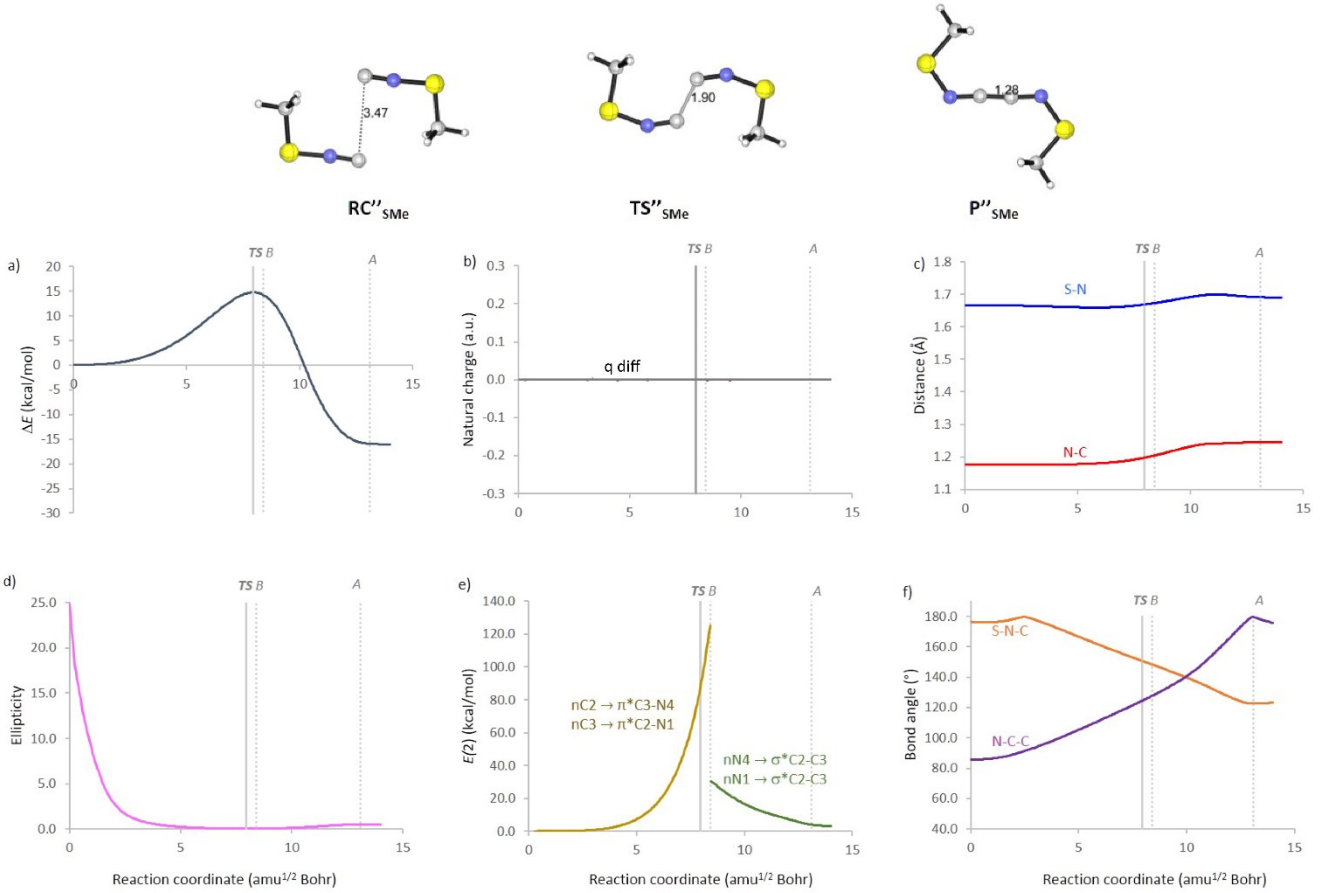


Figure S9. Computed potential energy profile (a), evolution of the total NBO-charges of the two monomers (b), the representative distances (Å,c), the ellipticity at the BCP of the C2-C3 bond (d), stabilizing orbital charge transfer interaction E(2) values (kcal mol^{-1},e) and the representative bond angles (°,f) along the reaction coordinate of the dimerization of MeS-NC (conformation of **TS''$_{SMe}$**) at the wB97X-D/def2-SVPD theoretical level. Numeration: left unit: MeS-N1-C2; right unit: C3-N4-SMe

5. Homodimerization of Me_3PN-NC

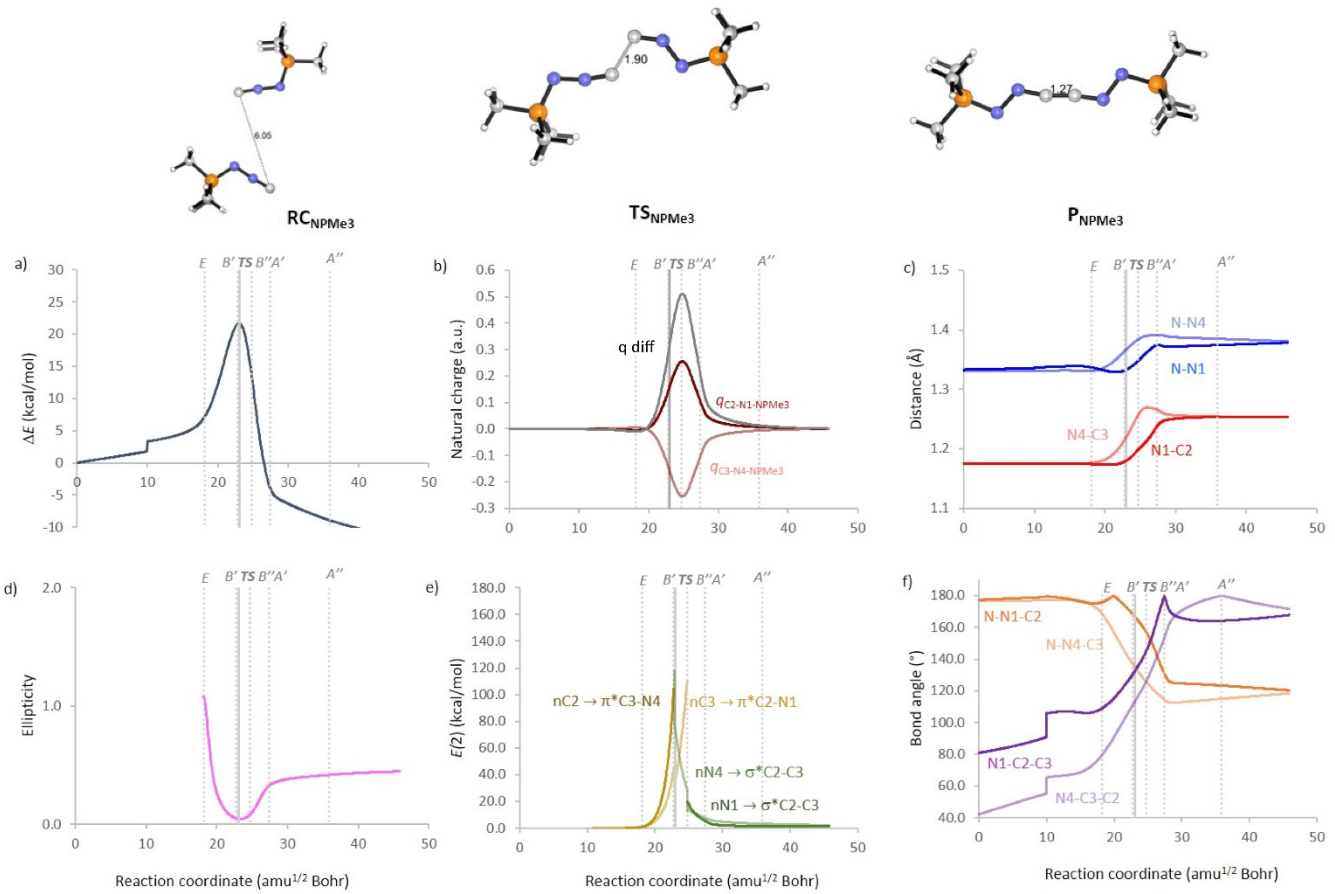


Figure S10. Computed potential energy profile (a), evolution of the total NBO-charges of the two monomers (b), the representative distances (Å,c), the ellipticity at the BCP of the C2-C3 bond (d), stabilizing orbital charge transfer interaction E(2) values (kcal mol^{-1},e) and the representative bond angles (°,f) along the reaction coordinate of the dimerization of Me_3PN-NC (conformation of $\mathbf{TS_{Me3PN\text{-}NC)}}$ at the wB97X-D/def2-SVPD theoretical level. Numeration: left unit: Me_3PN-N1-C2; right unit: C3-N4-$PNMe_3$

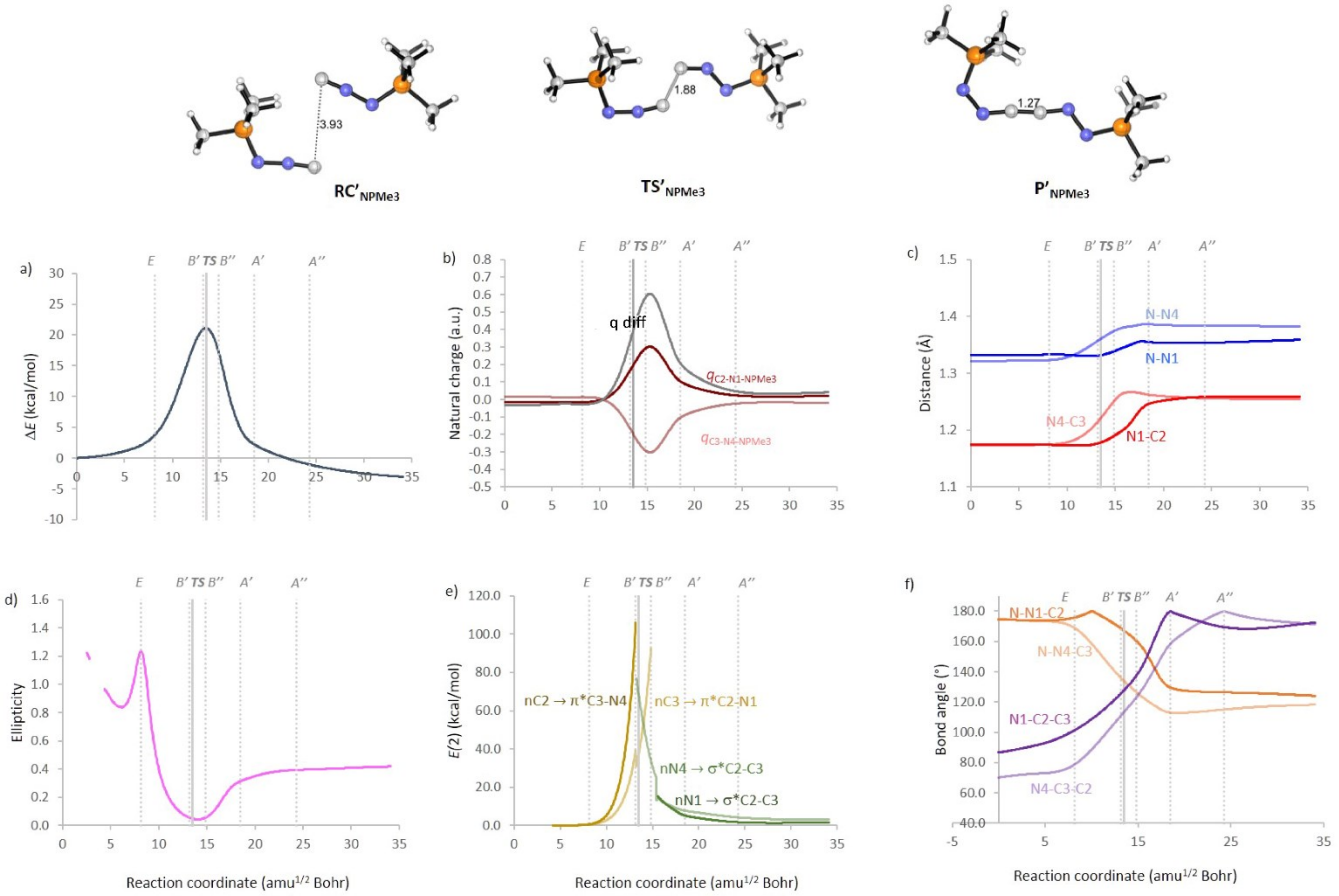


Figure S11. Computed potential energy profile (a), evolution of the total NBO-charges of the two monomers (b), the representative distances (Å,c), the ellipticity at the BCP of the C2-C3 bond (d), stabilizing orbital charge transfer interaction E(2) values (kcal mol^{-1},e) and the representative bond angles (°,f) along the reaction coordinate of the dimerization of Me_3PN-NC (conformation of **TS'$_{Me3PN-NC)}$** at the wB97X-D/def2-SVPD theoretical level. Numeration: left unit: Me_3PN-N1-C2; right unit: C3-N4-$PNMe_3$

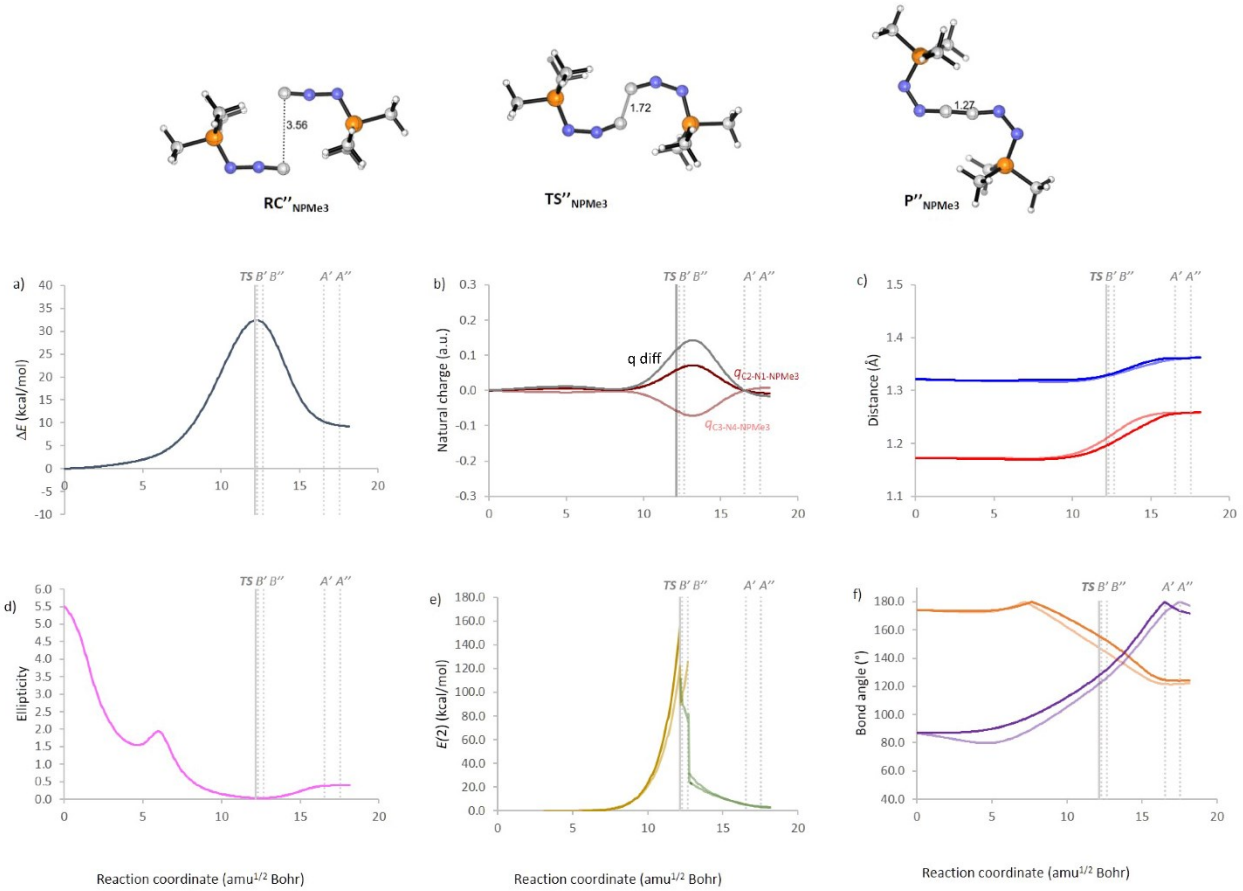


Figure S12. Computed potential energy profile (a), evolution of the total NBO-charges of the two monomers (b), the representative distances (Å,c), the ellipticity at the BCP of the C2-C3 bond (d), stabilizing orbital charge transfer interaction E(2) values (kcal mol^{-1},e) and the representative bond angles (°,f) along the reaction coordinate of the dimerization of Me_3PN-NC (conformation of **TS''$_{Me3PN-NC)}$** at the wB97X-D/def2-SVPD theoretical level. Numeration: left unit: Me_3PN-N1-C2; right unit: C3-N4-$PNMe_3$

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7. Cartesian coordinates

$RC_{F\text{-}LE}$
SCF = -384.649883517
Num. Imaginary Freq = 0

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N	1.790673	-0.420913	-0.000004
F	2.524948	0.633984	0.000034

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N	2.052058	0.377530	0.000023
C	-0.902978	-0.856911	-0.000037
N	-1.927155	-0.281391	-0.000019
F	2.461869	-0.840476	-0.000022
F	-3.045481	0.353533	0.000002

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SCF = -384.649564978

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C	-2.406593	-0.425581	-0.000007
H	-1.769619	-1.319791	0.000017
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H	2.260921	1.337022	-0.000019
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H	3.548964	0.008070	-0.883735
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O	-2.832699	0.531516	0.005113
C	2.846625	0.899443	-0.000065
H	3.908440	1.159823	0.012694
H	2.358033	1.283900	-0.905224
H	2.334200	1.291090	0.888629
C	-2.846633	-0.899439	-0.000049
H	-2.334234	-1.291054	0.888674
H	-3.908450	-1.159810	0.012698
H	-2.358023	-1.283937	-0.905182

P_{OMe}
SCF = -415.335059225

C	0.631012	0.033868	0.000000
N	1.801878	0.462502	-0.000001
C	-0.635644	-0.115930	0.000000
N	-1.820592	-0.503251	0.000001
O	-2.750357	0.497310	-0.000001
O	2.776928	-0.491005	0.000001
C	-4.055897	-0.051864	0.000001
H	-4.735718	0.806537	-0.000001
H	-4.218896	-0.662592	-0.899171
H	-4.218895	-0.662588	0.899175
C	4.052397	0.126652	0.000000
H	4.181634	0.745436	0.899066
H	4.777459	-0.693780	0.000002
H	4.181634	0.745434	-0.899067

P'_{OMe}
SCF = -415.332249518

C	-0.419903	-0.130987	0.000009
N	-1.536573	0.421638	0.000030
C	0.817958	-0.447272	-0.000015
N	1.918008	-1.042874	-0.000034
O	3.070789	-0.334952	-0.000063
O	-2.603328	-0.433206	0.000059
C	2.946624	1.075420	-0.000071
H	3.971352	1.458126	-0.000096
H	2.410826	1.419052	-0.899208
H	2.410865	1.419065	0.899083
C	-3.814225	0.300939	0.000083
H	-3.886627	0.928918	-0.899163
H	-4.612293	-0.448778	0.000106
H	-3.886585	0.928927	0.899327

P''_{OMe}
SCF = -415.329704436

C	0.574280	0.281028	0.000946
N	1.547735	1.064734	0.000219
C	-0.574280	-0.281032	0.000944
N	-1.547737	-1.064735	0.000212
O	-2.808570	-0.567558	-0.000478
O	2.808569	0.567559	-0.000472
C	-2.925478	0.843717	-0.000379
H	-4.000099	1.047158	-0.001251
H	-2.456813	1.273792	0.899094
H	-2.455311	1.274056	-0.898940
C	2.925480	-0.843716	-0.000382
H	2.455314	-1.274050	-0.898946
H	4.000102	-1.047155	-0.001254
H	2.456816	-1.273796	0.899088

RC_{SMe}
SCF = -1061.24542576

C	-0.939453	-1.487677	-0.001205
N	-1.773930	-0.656632	-0.000721
C	0.939639	1.487924	-0.001021
N	1.773999	0.656763	-0.000593
S	2.824403	-0.636854	-0.000085
S	-2.824514	0.636839	-0.000136
C	4.389724	0.264843	0.001311
H	5.169182	-0.509475	0.001741
H	4.487944	0.879510	-0.901383
H	4.486555	0.879112	0.904426
C	-4.389712	-0.265068	0.001393
H	-4.486386	-0.879345	0.904520
H	-5.169274	0.509145	0.001883
H	-4.487923	-0.879753	-0.901290

RC'_{SMe}
SCF = -1061.24816371

C	0.754570	1.565862	-0.003121
N	1.562823	0.710764	-0.001723
C	-0.812124	-1.629074	-0.001126
N	-1.838039	-1.051633	-0.000481
S	-3.316547	-0.281532	0.000380
S	2.588831	-0.602874	0.000176
C	-2.757390	1.435496	0.001524
H	-3.678016	2.035297	0.002029
H	-2.169158	1.655022	0.899762
H	-2.169290	1.656286	-0.896486
C	4.166047	0.279369	0.001830

H	4.271012	0.892885	0.904581
H	4.935415	-0.504867	0.003220
H	4.273398	0.892033	-0.901219

RC''$_{SMe}$
SCF = -1061.24992123

C	0.686094	-1.593684	0.001025
N	1.726953	-1.045127	0.000291
C	-0.686096	1.593687	0.000891
N	-1.726954	1.045128	0.000167
S	-3.246054	0.359795	-0.000933
S	3.246054	-0.359796	-0.000817
C	-2.798159	-1.389081	0.000640
H	-3.757788	-1.924347	0.000258
H	-2.224051	-1.647737	-0.895962
H	-2.225485	-1.646480	0.898525
C	2.798162	1.389080	0.000642
H	2.225476	1.646535	0.898503
H	3.757791	1.924345	0.000239
H	2.224066	1.647682	-0.895984

TS$_{SMe}$
SCF = -1061.22420124
Num. Imaginary Freq = 1

C	0.629261	-0.727624	0.001227
N	1.815884	-0.562433	0.000857
C	-0.629314	0.727851	0.001081
N	-1.815929	0.562568	0.000632
S	-3.004195	-0.615859	0.000281
S	3.004265	0.615833	0.000360
C	-4.471374	0.431339	-0.001704
H	-5.326628	-0.258112	-0.001688
H	-4.509153	1.054683	0.899635
H	-4.507893	1.053104	-0.904187
C	4.471327	-0.431540	-0.001878
H	4.508040	-1.052796	-0.904703
H	5.326659	0.257815	-0.001203
H	4.508776	-1.055392	0.899123

TS'$_{SMe}$
SCF = -1061.22548400
Num. Imaginary Freq = 1

C	-0.372071	0.617619	0.003646
N	-1.574296	0.575990	0.001941
C	0.675474	-0.982840	0.002598
N	1.867159	-1.028058	-0.001057
S	3.376000	-0.319576	-0.000820
S	-2.810022	-0.557900	-0.000340
C	2.921664	1.426677	-0.000698
H	3.876971	1.968498	-0.001235
H	2.345994	1.684227	-0.897891
H	2.346756	1.684461	0.896916
C	-4.235233	0.545025	-0.002026
H	-4.249355	1.166861	-0.905167
H	-5.117288	-0.109704	0.000272
H	-4.247777	1.170855	0.898357

TS''$_{SMe}$
SCF = -1061.22642510
Num. Imaginary Freq = 1

C	-0.407208	-0.856012	-0.001162
N	-1.589418	-1.044265	-0.000468
C	0.407219	0.856032	-0.001072
N	1.589430	1.044278	-0.000365
S	3.154020	0.465013	0.001092
S	-3.154016	-0.465023	0.000976
C	2.876219	-1.317049	-0.000646
H	3.883530	-1.755012	-0.001014
H	2.332735	-1.636826	0.896591
H	2.332892	-1.634941	-0.898649
C	-2.876240	1.317042	-0.000646
H	-2.332869	1.634992	-0.898603
H	-3.883557	1.754992	-0.001058
H	-2.332814	1.636780	0.896640

P$_{SMe}$
SCF = -1061.27362430

C	0.631057	0.099273	-0.000653
N	1.814428	0.486342	-0.000382
C	-0.631067	-0.099374	-0.000659
N	-1.814450	-0.486404	-0.000427
S	-3.096552	0.632640	-0.000156
S	3.096588	-0.632630	-0.000253
C	-4.453981	-0.548164	0.001001
H	-5.379016	0.043869	0.001066
H	-4.422179	-1.173672	-0.899094
H	-4.421465	-1.172748	0.901713
C	4.453946	0.548256	0.001068
H	4.421387	1.172715	0.901863
H	5.379018	-0.043718	0.001055
H	4.422106	1.173883	-0.898943

P'$_{SMe}$
SCF = -1061.27439608

C	0.409844	-0.135016	-0.000291
N	1.533749	0.400674	-0.000265
C	-0.802801	-0.536986	-0.000175
N	-1.917213	-1.094360	0.000084
S	-3.385719	-0.268292	0.000254
S	2.944754	-0.556108	-0.000141
C	-2.919555	1.473239	-0.000203
H	-3.857823	2.043508	-0.000090
H	-2.338942	1.723571	0.898266
H	-2.339381	1.723204	-0.899056
C	4.152367	0.777117	0.000443
H	4.047956	1.393891	0.901141
H	5.140452	0.297532	0.000505
H	4.048298	1.394375	-0.899960

P''$_{SMe}$
SCF = -1061.27552114

C	-0.539902	0.340574	0.000217
N	-1.541517	1.081021	0.000069
C	0.539905	-0.340584	0.000180
N	1.541522	-1.081026	-0.000041
S	3.125484	-0.493170	-0.000261
S	-3.125482	0.493174	-0.000144
C	2.928862	1.298792	0.000190
H	3.942972	1.719161	0.000019
H	2.393143	1.635568	-0.897948
H	2.393616	1.635151	0.898768
C	-2.928872	-1.298790	0.000190
H	-2.393604	-1.635208	0.898733
H	-3.942984	-1.719153	0.000018
H	-2.393177	-1.635513	-0.897983

RC$_{NPMe3}$
SCF = -1216.48228982

C	2.789001	2.919358	-0.001622
N	2.780119	1.744468	0.000556
C	-1.290694	-1.541436	-0.003327
N	-2.022497	-0.622216	-0.003087
N	-2.802509	0.458602	-0.003008
N	2.691743	0.416578	0.003191
P	4.115155	-0.339636	0.000532
P	-4.378909	0.115785	0.000333
C	5.159740	0.026511	-1.442021
H	5.305744	1.114778	-1.486942
H	6.136800	-0.470815	-1.374649
H	4.636110	-0.295067	-2.351060
C	5.167288	0.030625	1.436560
H	4.648313	-0.288117	2.349260
H	6.143896	-0.467102	1.365646
H	5.313736	1.118990	1.477462
C	3.736124	-2.097594	0.004069
H	3.135263	-2.329080	-0.883963
H	4.660275	-2.690151	0.002036
H	3.140777	-2.326737	0.896407
C	-4.938050	-0.837301	1.443211
H	-6.005270	-1.088451	1.377078
H	-4.346816	-1.762539	1.487433
H	-4.744584	-0.253820	2.352129
C	-5.230625	1.700712	-0.000346
H	-4.931606	2.261591	-0.894258
H	-6.318012	1.550425	0.001808
H	-4.928414	2.264078	0.890925
C	-4.943213	-0.841345	-1.437853
H	-6.010160	-1.092404	-1.367147
H	-4.753106	-0.260377	-2.349087
H	-4.352055	-1.766651	-1.481649

RC'$_{NPMe3}$
SCF = -1216.49089532

C	0.372711	-1.260228	0.000088
N	1.248347	-0.478820	0.000037
C	-1.090705	2.382862	-0.000138
N	-2.152972	1.880641	-0.000126
N	-3.407157	1.432987	-0.000119
N	2.154392	0.483468	-0.000028
P	3.694975	0.013838	0.000042
P	-3.584829	-0.172010	-0.000036
C	4.191181	-0.975860	1.441601
H	3.559441	-1.874010	1.478703
H	5.246214	-1.275721	1.381672
H	4.019449	-0.387456	2.351708
C	4.191244	-0.976081	-1.441344
H	4.019552	-0.387815	-2.351548
H	5.246275	-1.275933	-1.381324
H	3.559506	-1.874237	-1.478336
C	4.652457	1.536543	-0.000054
H	4.386394	2.117212	0.891636
H	5.727680	1.315622	-0.000018
H	4.386427	2.117079	-0.891841
C	-2.893796	-1.034447	1.438101
H	-3.126603	-2.107423	1.399534
H	-1.801780	-0.914451	1.414981
H	-3.301291	-0.589275	2.354353
C	-5.370528	-0.423923	-0.000048
H	-5.794691	0.051583	-0.892767
H	-5.605671	-1.496104	-0.000001
H	-5.794716	0.051667	0.892615

C	-2.893753	-1.034598	-1.438061
H	-3.126534	-2.107575	-1.399373
H	-3.301242	-0.589542	-2.354371
H	-1.801741	-0.914572	-1.414935

RC''$_{NPMe3}$
SCF = -1216.50830105

C	0.206240	-1.761751	-0.000004
N	1.362047	-1.565652	-0.000008
C	-0.213052	1.778217	0.000000
N	-1.367630	1.574477	-0.000002
N	-2.685248	1.474554	-0.000004
N	2.680193	-1.474238	-0.000013
P	3.316612	0.017238	0.000002
P	-3.314507	-0.019984	-0.000001
C	2.906568	1.037384	-1.438520
H	1.833638	1.272547	-1.385483
H	3.474551	1.977650	-1.416312
H	3.133147	0.479964	-2.355824
C	2.906557	1.037357	1.438539
H	3.133128	0.479920	2.355835
H	3.474539	1.977625	1.416352
H	1.833627	1.272521	1.385498
C	5.095404	-0.277747	0.000005
H	5.358497	-0.857624	-0.892978
H	5.638965	0.675740	0.000012
H	5.358492	-0.857635	0.892982
C	-2.902139	-1.037896	1.439465
H	-3.465131	-1.981127	1.415828
H	-1.827999	-1.267349	1.389332
H	-3.134458	-0.481408	2.355914
C	-5.094891	0.265622	0.000000
H	-5.361501	0.843838	-0.893008
H	-5.632776	-0.691100	0.000001
H	-5.361499	0.843839	0.893008
C	-2.902142	-1.037902	-1.439463
H	-3.465135	-1.981133	-1.415821
H	-3.134465	-0.481418	-2.355914
H	-1.828003	-1.267355	-1.389332

TS$_{NPMe3}$
SCF = -1216.44792234
Num. Imaginary Freq = 1

C	-0.863902	-1.665623	0.000005
N	-1.953482	-1.118872	0.000085
C	0.575776	-0.432148	-0.000380
N	1.745434	-0.586102	-0.000414
N	2.993980	-1.052168	-0.000512
N	-2.390500	0.175749	-0.000042
P	-3.997329	0.252093	0.000106
P	4.111285	0.115748	-0.000067
C	-4.821450	-0.509658	-1.435456
H	-4.509177	-1.561892	-1.477253
H	-5.916225	-0.452180	-1.362665
H	-4.478547	-0.007459	-2.348990
C	-4.821174	-0.509246	1.436045
H	-4.478093	-0.006783	2.349366
H	-5.915963	-0.451781	1.363449
H	-4.508901	-1.561470	1.478087
C	-4.419997	2.005908	-0.000106
H	-3.985951	2.472778	-0.892699
H	-5.509510	2.141132	-0.000021
H	-3.985778	2.473042	0.892266
C	4.047937	1.220919	1.441040
H	4.798007	2.020525	1.375069
H	3.043239	1.663905	1.482466
H	4.207371	0.629032	2.351127
C	5.699828	-0.730463	-0.000302
H	5.760159	-1.364517	-0.893283
H	6.522553	-0.003915	0.000053
H	5.760028	-1.365244	0.892172
C	4.048050	1.221943	-1.440393
H	4.798132	2.021488	-1.373818
H	4.207528	0.630691	-2.350886
H	3.043364	1.664977	-1.481568

TS'$_{NPMe3}$
SCF = -1216.45729249
Num. Imaginary Freq = 1

C	0.110159	-0.491518	0.000045
N	1.330737	-0.453813	0.000050
C	-0.685209	1.206714	-0.000077
N	-1.835180	1.463007	-0.000107
N	-3.167031	1.456022	-0.000126
N	2.243148	0.555504	-0.000014
P	3.758893	0.012529	0.000039
P	-3.724381	-0.074962	-0.000038
C	4.230017	-1.003191	1.436956
H	3.552428	-1.866768	1.474080
H	5.269200	-1.353352	1.370422
H	4.091326	-0.410315	2.349926
C	4.230042	-1.003400	-1.436722
H	4.091372	-0.410656	-2.349781
H	5.269222	-1.353557	-1.370117
H	3.552450	-1.866979	-1.473735
C	4.809988	1.477326	-0.000058
H	4.581677	2.073458	0.891876

H	5.870420	1.193327	-0.000030
H	4.581689	2.073331	-0.892081
C	-3.195231	-1.051392	1.432120
H	-3.632972	-2.058787	1.405970
H	-2.098106	-1.127716	1.376853
H	-3.486248	-0.535654	2.355588
C	-5.520887	0.060966	-0.000080
H	-5.834012	0.615407	-0.893206
H	-5.978862	-0.936575	-0.000020
H	-5.834043	0.615528	0.892960
C	-3.195178	-1.051575	-1.432052
H	-3.632921	-2.058966	-1.405790
H	-3.486160	-0.535955	-2.355598
H	-2.098055	-1.127892	-1.376735

TS''$_{NPMe3}$
SCF = -1216.45662029

C	-0.060423	-0.628377	0.000010
N	-1.076900	-1.260299	0.000014
C	0.140664	1.081414	0.000008
N	1.228612	1.613477	0.000005
N	2.544878	1.443259	0.000001
N	-2.396770	-1.419966	0.000019
P	-3.286894	-0.053467	-0.000001
P	3.228031	-0.035092	-0.000001
C	-3.069797	1.027737	1.442163
H	-2.047574	1.428503	1.405671
H	-3.795018	1.853279	1.420510
H	-3.202645	0.437209	2.357368
C	-3.069776	1.027702	-1.442188
H	-3.202600	0.437151	-2.357380
H	-3.795004	1.853239	-1.420571
H	-2.047556	1.428478	-1.405684
C	-4.993884	-0.636758	-0.000004
H	-5.158246	-1.252686	0.892445
H	-5.687776	0.213961	-0.000007
H	-5.158243	-1.252690	-0.892451
C	2.973679	-1.110365	-1.449924
H	3.704345	-1.932021	-1.447729
H	1.954337	-1.511796	-1.422021
H	3.101603	-0.507474	-2.358115
C	4.992778	0.363050	0.000006
H	5.220636	0.959938	0.891276
H	5.595594	-0.554774	-0.000021
H	5.220630	0.959989	-0.891230
C	2.973670	-1.110381	1.449909
H	3.704377	-1.932000	1.447744
H	3.101527	-0.507484	2.358105
H	1.954349	-1.511861	1.421964

P$_{NPMe3}$
SCF = -1216.50020230

C	-0.630642	-0.201802	-0.000100
N	-1.859391	-0.450540	-0.000076
C	0.640946	-0.133959	-0.000118
N	1.850317	0.196575	-0.000113
N	2.835157	-0.767465	-0.000172
N	-2.742092	0.611334	-0.000022
P	-4.266699	0.084300	0.000095
P	4.276634	-0.033934	-0.000066
C	-4.744400	-0.926321	-1.437310
H	-4.069057	-1.791612	-1.472806
H	-5.785209	-1.271432	-1.370010
H	-4.603388	-0.334278	-2.350471
C	-4.744227	-0.926150	1.437679
H	-4.603083	-0.334004	2.350753
H	-5.785051	-1.271251	1.370558
H	-4.068895	-1.791449	1.473186
C	-5.305854	1.558514	0.000077
H	-5.073043	2.152761	-0.892023
H	-6.369029	1.284483	0.000172
H	-5.072912	2.152873	0.892069
C	4.594990	1.036124	1.437523
H	5.570003	1.537634	1.369522
H	3.793493	1.786002	1.471829
H	4.547315	0.429557	2.350802
C	5.522871	-1.337014	-0.000243
H	5.383363	-1.959435	-0.892638
H	6.532282	-0.905225	-0.000145
H	5.383312	-1.959722	0.891942
C	4.594998	1.036538	-1.437345
H	5.570009	1.538031	-1.369187
H	4.547336	0.430235	-2.350799
H	3.793497	1.786422	-1.471442

P'$_{NPMe3}$
SCF = -1216.49574354

C	0.125581	0.853955	-0.000053
N	1.196713	0.199748	0.000002
C	-1.050146	1.345429	-0.000099
N	-2.137942	1.978400	-0.000155
N	-3.362169	1.388842	-0.000132
N	2.389159	0.898066	-0.000029
P	3.660396	-0.092060	0.000048
P	-3.505110	-0.231253	-0.000025
C	3.791973	-1.204257	1.437130
H	2.880624	-1.815902	1.471930

H	4.672372	-1.858007	1.370870
H	3.842840	-0.598456	2.350714
C	3.792006	-1.204439	-1.436890
H	3.842898	-0.598754	-2.350549
H	4.672401	-1.858184	-1.370525
H	2.880656	-1.816086	-1.471635
C	5.118741	0.968398	-0.000002
H	5.089833	1.606217	0.891882
H	6.036540	0.365859	0.000042
H	5.089848	1.606110	-0.891963
C	-2.821931	-1.116537	1.441516
H	-3.083219	-2.183498	1.402601
H	-1.730163	-1.005412	1.442739
H	-3.229235	-0.667775	2.356355
C	-5.286111	-0.526966	-0.000031
H	-5.719420	-0.057146	-0.891337
H	-5.503030	-1.603366	0.000040
H	-5.719446	-0.057022	0.891196
C	-2.821889	-1.116732	-1.441427
H	-3.083181	-2.183688	-1.402377
H	-3.229163	-0.668092	-2.356338
H	-1.730121	-1.005610	-1.442632
H	-3.081398	-0.504423	2.357688
C	-5.030917	0.291136	-0.000010
H	-5.288014	0.875822	-0.891482
H	-5.585824	-0.656246	-0.000004
H	-5.288019	0.875836	0.891452
C	-2.898086	-1.076488	-1.439410
H	-3.544025	-1.965670	-1.421999
H	-3.081334	-0.504436	-2.357682
H	-1.847577	-1.391828	-1.412157

P''$_{NPMe3}$
SCF = -1216.49355287

C	0.375295	-0.329647	-0.000014
N	1.054357	-1.389657	-0.000027
C	-0.457503	0.634644	-0.000005
N	-1.236395	1.622982	0.000001
N	-2.592734	1.480700	-0.000001
N	2.416111	-1.425119	-0.000026
P	3.272263	-0.041840	0.000001
P	-3.251144	-0.011844	-0.000001
C	3.058905	1.056509	-1.440699
H	2.038599	1.459808	-1.439254
H	3.778008	1.886813	-1.402520
H	3.214379	0.473194	-2.356980
C	3.058890	1.056457	1.440738
H	3.214358	0.473109	2.357000
H	3.777990	1.886764	1.402596
H	2.038581	1.459753	1.439300
C	4.995494	-0.578046	0.000002
H	5.172059	-1.191809	-0.891556
H	5.671715	0.286932	0.000014
H	5.172053	-1.191828	0.891548
C	-2.898100	-1.076471	1.439424
H	-3.544009	-1.965675	1.421995
H	-1.847581	-1.391778	1.412207