

On the Origin of Ionicity in Ionic Liquids.

Ion Pairing versus Charge Transfer

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SUPPORTING INFORMATION

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1. Potential form applied in the MD simulations:

$$\begin{aligned} E_{pot} = & \sum_{bonds} K_r (r - r_0)^2 \\ & + \sum_{angles} K_\theta (\theta - \theta_0)^2 \\ & + \sum_{dihedrals} K_\phi [1 + d \cos(n\phi)] \\ & + \sum_{improper} K_\chi (\chi - \chi_0)^2 \\ & + \sum_{i < j} \left\{ 4 \epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] + \frac{C q_i q_j}{\epsilon r_{ij}} \right\} \end{aligned}$$

2. σ -values of the sodium in the different setups, and the corresponding cut-off values.

sizeNa	σ	cut-off
100%	3.33 Å	10 Å
150%	4.95 Å	15 Å
200%	6.66 Å	17 Å

3. Calculated charges for the IL ion pairs.

Ionic Liquid	Charge Transfer					
	NBO	LOWDIN	MULLIKEN	BLOECHL	RESP	AIM
Bmim NTf ₂	0.03592	0.45347	0.07737	0.23781	0.35219	0.05226
Bmim PF ₆	0.033115	0.434225	0.096935	0.144245	0.17368	0.03862
Bmim BF ₄	0.042785	0.36069	0.10866	0.17075	0.186985	0.05204
Bmim TfO	0.059915	0.44705	0.12067	0.204515	0.16074	0.0765
Bmim TFA	0.096925	0.44825	0.15714	0.20758	0.18803	0.10595
Mmim NTf ₂	0.05171	0.438745	0.102625	0.214635	0.25456	0.0712
Emim NTf ₂	0.03429	0.42191	0.083305	0.23522	0.31	0.04838
Bmim NTf ₂	0.03592	0.45347	0.07737	0.23781	0.35219	0.05226
Hmim NTf ₂	0.042675	0.42475	0.081745	0.28509	0.291515	0.05787
Omim NTf ₂	0.056025	0.54187	0.09121	0.345055	0.2979	0.06303
Bmim NTf ₂	0.03592	0.45347	0.07737	0.23781	0.35219	0.05226
bmpyr NTf ₂	0.037495	0.40759	0.080735	0.293505	0.280235	0.06025
bpy NTf ₂	0.052215	0.410265	0.09203	0.30552	0.240385	0.0698
N ₁₁₁₄ NTf ₂	0.0345	0.4819	0.07379	0.27153	0.25228	0.05444

Table S1. Charge transfer within ion pairs in the gas phase on BLYP-D3/def2-tzvp optimized structures, obtained with Turbomole 6.5. Charges calculated as follows: NBO: Turbomole BLYP-D3/def2-tzvp level; LOWDIN, MULLIKEN, BLOECHL, RESP: CP2k program package BLYP-D3/TZVP-MOLOPT-GTH/GTH-BLYP; AIM: AIMAll 2.6 wavefunction obtained from Turbomole optimized structures.

Ionic Liquid	Charge Transfer			
	LOWDIN	MULLIKEN	BLOECHL	RESP
Bmim NTf ₂	0.337045	0.057755	0.17761	0.26002
Bmim PF ₆	0.270365	0.064535	0.09004	0.120375
Bmim BF ₄	0.23212	0.07527	0.12289	0.132745
Bmim TfO	0.335855	0.084775	0.157755	0.12002
Bmim TFA	0.33418	0.113365	0.156045	0.16483
Mmim NTf ₂	0.311335	0.070565	0.16535	0.18938
Emim NTf ₂	0.285875	0.059225	0.149515	0.22065
Bmim NTf ₂	0.337045	0.057755	0.17761	0.26002
Hmim NTf ₂	0.308855	0.05626	0.21756	0.23243
Omim NTf ₂	0.405735	0.06634	0.27773	0.34448
Bmim NTf ₂	0.337045	0.057755	0.17761	0.26002
bmpyr NTf ₂	0.32227	0.062855	0.25413	0.228275
bpy NTf ₂	0.308585	0.06862	0.25141	0.220535
N ₁₁₁₄ NTf ₂	0.36469	0.05442	0.20967	0.21

Table S2. Charge transfer within ion pairs solvated by the COSMO model. Optimized structures obtained with Turbomole 6.5 on the TPSS-D3/def2-tzvp + COSMO level. Charges calculated by the CP2K program package on the optimized structures, using the TPSS-D3 functional, TZVP-MOLOPT-GTH basis set, and GTH-PBE pseudopotentials.

Ionic Liquid	Charge Transfer							
	Turbomole				Turbomole + Cosmo			
	BLYP-D3/def2-tzvp optimized structures				BLYP-D3/def2-tzvp optimized structures			
	NBO	LOWDIN	MULL	AIM	NBO	LOWDIN	MULL	AIM
Bmim NTf ₂	0.03592	0.185415	0.134775	0.05226	0.0172	0.120945	0.07918	0.019985
Bmim PF ₆	0.033115	0.17606	0.150145	0.038615	0.0153	0.104725	0.084745	0.008195
Bmim BF ₄	0.042785	0.114945	0.131915	0.05204	0.018515	0.050965	0.0611	0.019165
Bmim TfO	0.059915	0.190465	0.17254	0.076495	0.02373	0.112395	0.08771	0.031905
Bmim TFA	0.096925	0.205715	0.20395	0.105945	0.044455	0.1152	0.112	0.046695
Mmim NTf ₂	0.05171	0.183425	0.153545	0.0712	0.02349	0.11232	0.084455	0.03147
Emim NTf ₂	0.03429	0.184725	0.13955	0.048375	0.01522	0.11474	0.073035	0.01583
Bmim NTf ₂	0.03592	0.185415	0.134775	0.05226	0.0172	0.120945	0.07918	0.019985
Hmim NTf ₂	0.042675	0.177725	0.13547	0.05787	0.0198	0.113545	0.075735	0.02304
Omim NTf ₂	0.056025	0.2099	0.162035	0.063025	0.028405	0.142335	0.102075	0.02403
Bmim NTf ₂	0.03592	0.185415	0.134775	0.05226	0.0172	0.120945	0.07918	0.019985
bmpyr NTf ₂	0.037495	0.16397	0.138195	0.060245	0.018845	0.105185	0.08072	0.030115
bpy NTf ₂	0.052215	0.192885	0.138665	0.069795	0.024665	0.119565	0.07574	0.030125
N ₁₁₁₄ NTf ₂	0.0345	0.17057	0.13665	0.05444	0.01641	0.10867	0.08372	0.04409

Table S3. Comparison of charge transfer within ion pairs in the gas phase on BLYP-D3/def2-tzvp optimized structures (left block) and on BLYP-D3/def2-tzvp+COSMO (right block) optimized structures, obtained with Turbomole 6.5. Charges calculated as follows: NBO, LOWDIN, MULL: Turbomole BLYP-D3/def2-tzvp level (left block) and BLYP-D3/def2-tzvp+COSMO (right block); AIM: AIMAll 2.6 wavefunction obtained from Turbomole optimized structures (left block) and the Turbomole+COSMO optimized structures.

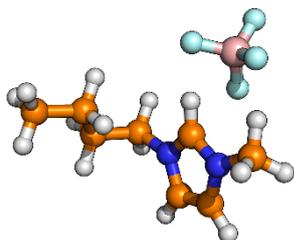
Ionic Liquid	Charge Transfer		
	NBO	LOWDIN	MULLIKEN
Bmim NTf ₂	0.01312	0.102605	0.062645
Bmim PF ₆	0.01077	0.082355	0.065035
Bmim BF ₄	0.01406	0.04083	0.050515
Bmim TfO	0.01934	0.100925	0.074395
Bmim TFA	0.03887	0.100445	0.094305
Mmim NTf ₂	0.01765	0.095425	0.069355
Emim NTf ₂	0.010535	0.09166	0.056675
Bmim NTf ₂	0.01312	0.102605	0.062645
Hmim NTf ₂	0.01468	0.09114	0.060685
Omim NTf ₂	0.02209	0.11914	0.080765
Bmim NTf ₂	0.01312	0.102605	0.062645
bmpyr NTf ₂	0.016055	0.093165	0.067555
bpy NTf ₂	0.01979	0.10454	0.05872
N ₁₁₁₄ NTf ₂	0.01214	0.09431	0.06866

Table S4. Charge transfer within ion pairs solvated by the COSMO model. Optimized structures obtained with Turbomole 6.5 on the TPSS-D3/def2-tzvp + COSMO level. Charges calculated as follows: NBO, LOWDIN, MULL: Turbomole B3LYP-D3/def2-tzvp+COSMO level.

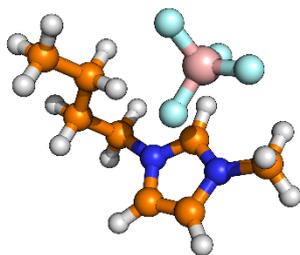
Ionic Liquid	Charge Transfer			
	LOWDIN	MULLIKEN	RESP	BLOECHL
Bmim NTf ₂	0.089835	0.03458	0.27443	0.189325
Bmim PF ₆	0.075505	0.0655	0.12181	0.088605
Bmim BF ₄	0.05928	0.09225	0.12912	0.116285
Bmim TfO	0.09855	0.101015	0.11003	0.15678
Bmim TFA	0.10408	0.113465	0.15657	0.144295

Table S4. Charge transfer within a small set of the ion pairs solvated by the COSMO model. Optimized structures obtained with Turbomole 6.5 on the TPSS-D3/def2-tzvp+COSMO level. Charges calculated as follows: LOWDIN, MULLIKEN, RESP, BLOECHL: CP2k program package B3LYP-D3/TZVP-GTH/GTH-BLYP level.

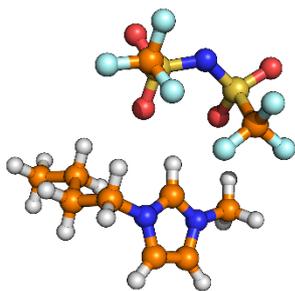
4. XYZ coordinates, and total energies of the tpss optimized structures.



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E(TPSS-D3/def2-TZVP)= -848.3425881221  
C 1.8508995 -0.5064095 -0.5254995  
C 0.1740407 -0.1386378 1.2918056  
C 1.7314846 0.5668203 -1.6116954  
C -0.4244695 -1.6345679 -0.2229872  
C -1.4240316 -1.5501824 0.7008440  
C 1.3991509 1.9629296 -1.0719098  
C -1.7778301 -0.2070928 2.8381992  
C 1.3680274 3.0199823 -2.1816831  
H 0.7517157 0.5816575 1.8466496  
H 2.5656701 -0.2172277 0.2477583  
H 2.1609128 -1.4642013 -0.9470555  
H -0.3254769 -2.2480833 -1.1036848  
H -2.3631259 -2.0736215 0.7793407  
H 2.6974321 0.5935075 -2.1312680  
H 0.9821720 0.2570128 -2.3513013  
H 0.4249267 1.9430362 -0.5656822  
H 2.1420811 2.2412336 -0.3128365  
H -2.1443921 -1.1034809 3.3392814  
H -1.0979164 0.3320448 3.4963866  
H -2.6146876 0.4299511 2.5467639  
H 2.3371114 3.0792629 -2.6910475  
H 0.6075329 2.7765575 -2.9325376  
H 1.1373161 4.0102328 -1.7752879  
N 0.5654991 -0.7490381 0.1672824  
N -1.0280672 -0.6116336 1.6394507  
B 2.5470867 -0.3162300 3.5062886  
F 2.2893091 -1.5391125 2.8454056  
F 3.5662795 -0.4839397 4.4593551  
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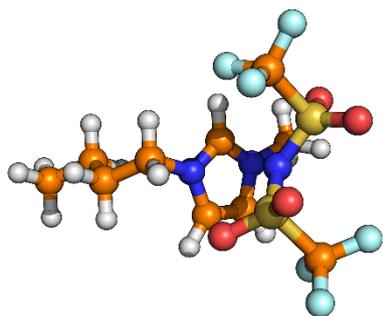
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C -0.8043791 -1.3749201 -0.6238018  
C -1.8493827 -1.2868368 0.2466887  
C 1.3956434 1.8788281 -1.0207639  
C -2.1767763 -0.2978476 2.5645390  
C 1.4281810 2.9871029 -2.0785881  
H 0.5449366 0.1401793 1.9190435  
H 2.3213636 -0.4416263 0.2349905  
H 1.9074115 -1.5960255 -1.0436683  
H -0.7420277 -1.7965951 -1.6138695  
H -2.8725746 -1.6143596 0.1595892  
H 2.6605172 0.4730276 -2.0881383  
H 0.9412592 0.2779067 -2.4167438  
H 0.4193826 1.8868084 -0.5241066  
H 2.1446557 2.0848662 -0.2442424  
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H -1.4996074 -0.0112228 3.3667859  
H -2.8152592 0.5472970 2.3037775  
H 2.4055211 3.0350250 -2.5748795  
H 0.6688724 2.8109710 -2.8490841  
H 1.2271910 3.9629816 -1.6248912  
N 0.2931904 -0.8073472 0.0015622  
N -1.3750774 -0.6660917 1.3883768  
B -1.4443863 3.0157959 1.4801817  
F -0.4288052 2.3722614 2.2359320  
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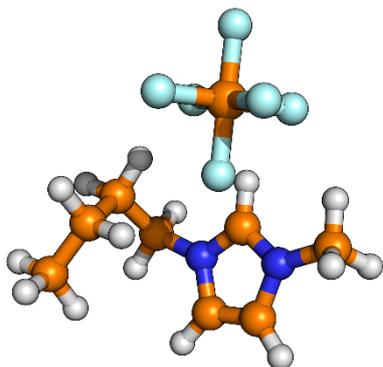
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F -3.2508857 0.0391619 6.4230225
F -3.1623244 1.4692617 4.7709692
F -0.8421335 -4.5216479 3.2849539
F -2.3922800 -3.7790567 4.6392688
F -1.7931229 -2.5914099 2.9052311
N -0.7347526 -1.3942644 5.6576271
O -0.4544323 1.0611428 6.0485206
O -0.6104244 0.2938761 3.6773586
O 0.9945251 -2.1973969 3.9209488
O 0.3373864 -3.6003273 5.8870628
S -0.0050897 -2.5889217 4.9058583
S -0.9279805 0.0871138 5.0833668
C -1.5515956 0.6937259 0.5244293
C 0.0447704 -1.2024172 0.9321287
C -0.8313902 1.9931532 0.1512426
C -0.7369627 -1.0590891 -1.1359542
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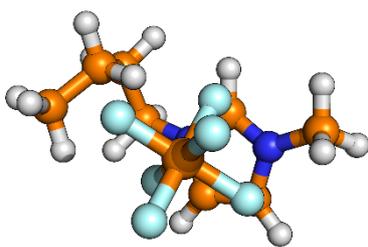
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H 0.9029438 3.6779629 -0.9571508  
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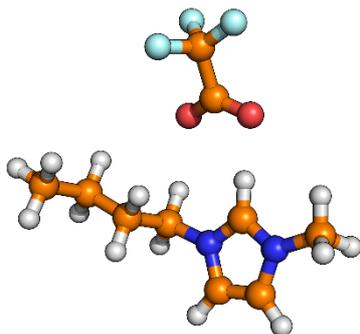
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F -2.0219028 -0.2266573 -2.4897706
F -3.8241922 -1.4107683 -1.6528244
F -3.7242218 -0.8836230 -3.9042158
P -3.6459831 -0.0263587 -2.5209259
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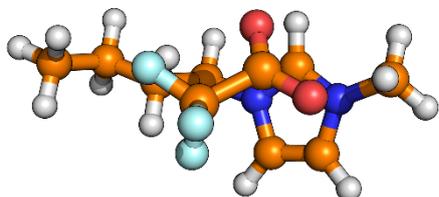
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F 0.2442217 -0.2240515 -3.2088241  
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F 2.1524250 -1.5327162 -3.2161698  
F 1.5951437 -0.2857996 -5.0798145  
P 1.8343004 0.0495711 -3.4989498  
C -0.2020223 1.1356730 1.2886788  
C -0.5786257 -0.7816322 -0.3107371  
C -1.0699545 2.0577900 0.4318390  
C 1.2434622 -0.9240983 0.9298807  
C 1.1766196 -2.0423692 0.1547188  
C -0.4386912 2.5277502 -0.8898019  
C -0.4187879 -2.8915416 -1.6306416  
C 0.8554346 3.3281257 -0.7083643  
H -1.4905814 -0.4291910 -0.7609294  
H -0.7117957 0.8895222 2.2243912  
H 0.7526629 1.6047219 1.5353897  
H 1.9738317 -0.6091326 1.6573092  
H 1.8410203 -2.8863899 0.0691828  
H -2.0382328 1.5778407 0.2410779  
H -1.2867079 2.9269566 1.0655954  
H -0.2401187 1.6730052 -1.5443041  
H -1.1823010 3.1470636 -1.4060936  
H -0.5401921 -3.8722501 -1.1687018  
H -1.3712697 -2.5453810 -2.0285681  
H 0.3250496 -2.9265518 -2.4263965  
H 0.6996933 4.1894818 -0.0469282  
H 1.6541724 2.7101159 -0.2851301  
H 1.2130534 3.6947650 -1.6750778  
N 0.1384336 -0.1483409 0.6260174  
N 0.0301567 -1.9347894 -0.6094284
```



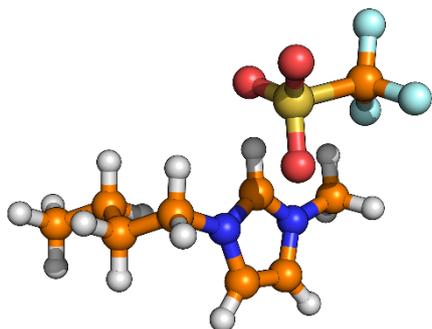
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==> bmim_tfa_tpss_inplane.xyz <==
E(TPSS-D3/def2-TZVP)= -950.1472708282
C -0.2728101 -0.9694597 -0.7374811
C -0.9980853 0.3056057 1.2792508
C 1.2215309 -1.2660299 -0.5932376
C -0.6355672 1.5546883 -0.5168040
C -0.9837725 2.3864970 0.5065748
C 1.5827601 -2.6059984 -1.2453490
C -1.6018841 2.0454514 2.9540751
C 3.0738306 -2.9341349 -1.1100003
H -1.0908436 -0.5513141 1.9563889
H -0.5600536 -0.8293271 -1.7819757
H -0.8582808 -1.7805872 -0.2996691
H -0.3859291 1.7637769 -1.5446676
H -1.0976798 3.4578963 0.5423280
H 1.8078604 -0.4527476 -1.0401373
H 1.4675898 -1.3026623 0.4751717
H 0.9841344 -3.3948706 -0.7731727
H 1.3047414 -2.5830176 -2.3075752
H -1.6391969 1.1781524 3.6128899
H -0.8639567 2.7602160 3.3213616
H -2.5854596 2.5144149 2.8972167
H 3.3095834 -3.8961546 -1.5776828
H 3.6913585 -2.1647075 -1.5886796
H 3.3660428 -2.9909858 -0.0549057
N -0.6551671 0.2644626 -0.0158498
N -1.2026370 1.5869131 1.6156516
C -0.2330833 -4.0802026 3.6742647
C -0.7842199 -2.9330177 2.7502982
F -0.4098532 -3.8543195 5.0036850
F -0.8174628 -5.2833504 3.4081900
F 1.1115829 -4.2517121 3.4875976
O -0.8177656 -3.2305228 1.5384717
O -1.0920097 -1.8666139 3.3409678

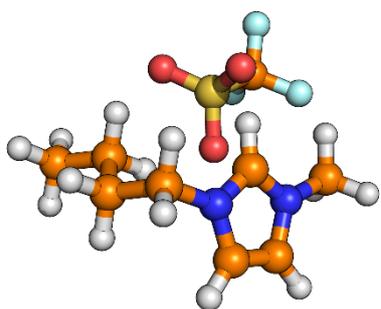
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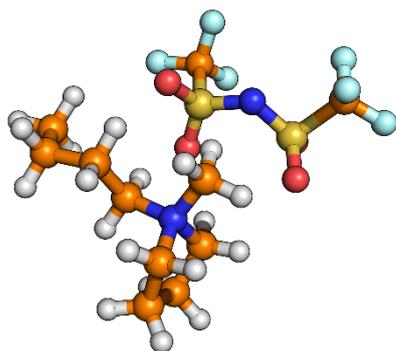
```
==> bmim_tfa_tpss_ontop.xyz <==  
E(TPSS-D3/def2-TZVP)= -950.1461711842  
C -0.2444280 -0.9805436 -0.6349440  
C -0.8344223 0.7570896 1.0648139  
C 1.2581236 -1.0415611 -0.9182191  
C -0.8388246 1.4694205 -1.0295982  
C -1.1352235 2.5277158 -0.2239568  
C 1.6927406 -2.4528831 -1.3339499  
C -1.3079115 2.8747639 2.2907247  
C 3.1932773 -2.5251538 -1.6396542  
H -0.7297122 0.1283791 1.9323205  
H -0.8334266 -1.2320736 -1.5210629  
H -0.5248121 -1.6668271 0.1673674  
H -0.7513811 1.3973266 -2.1014699  
H -1.3487276 3.5578926 -0.4578713  
H 1.5060251 -0.3264257 -1.7120757  
H 1.8002305 -0.7229246 -0.0205675  
H 1.4446243 -3.1597270 -0.5310840  
H 1.1203043 -2.7676577 -2.2171531  
H -1.6341605 2.2237850 3.1012545  
H -0.3437236 3.3305359 2.5289658  
H -2.0669335 3.6318112 2.0938874  
H 3.4891536 -3.5406069 -1.9239229  
H 3.4564871 -1.8516939 -2.4635548  
H 3.7842219 -2.2303842 -0.7648142  
N -0.6617300 0.3702399 -0.2050201  
N -1.1357644 2.0598745 1.0785362  
C 3.3198740 2.0200004 0.5152209  
C 2.2075720 2.1698985 1.6207939  
F 3.9642329 0.8215602 0.5303257  
F 2.7742086 2.1472564 -0.7365478  
F 4.2893729 2.9751062 0.6088712  
O 1.8498594 3.3547606 1.8093666  
O 1.8080499 1.0979733 2.1284672
```



```
==> bmim_tfo_tpss_inplane.xyz <==  
E(TPSS-D3/def2-TZVP)= -1385.514830610  
C 4.8673283 -0.2129818 -2.7947609  
F 4.7295799 -0.5569606 -1.4855356  
F 5.6839356 0.8642862 -2.8450636  
F 5.4954735 -1.2364368 -3.4175284  
O 2.7234894 1.2876608 -2.7753556  
O 2.4663927 -1.1043055 -3.3478572  
O 3.5282581 0.4437020 -4.9619059  
S 3.2008605 0.1512243 -3.5668354  
C -0.3061029 0.4774146 -1.8742076  
C 1.5682442 -0.3472467 -0.4332846  
C -1.7530521 0.0825531 -1.5656166  
C 0.4227368 1.3454386 0.4130694  
C 1.4038879 1.0192563 1.3012100  
C -1.9042099 -1.3331142 -0.9979191  
C 3.2713913 -0.7033240 1.3618659  
C -3.3668874 -1.7037426 -0.7235966  
H 1.9250272 -1.0967563 -1.1241714  
H -0.2485812 1.4806844 -2.3014369  
H 0.1671577 -0.2165538 -2.5715600  
H -0.3346605 2.1116324 0.4495059  
H 1.6610242 1.4402412 2.2596885  
H -2.1938435 0.8142755 -0.8755918  
H -2.3075478 0.1694265 -2.5078996  
H -1.4666649 -2.0523823 -1.7031122  
H -1.3299594 -1.4157816 -0.0660594  
H 2.9877022 -1.1029091 2.3362532  
H 3.5891618 -1.5120600 0.7060165  
H 4.0771391 0.0237939 1.4737434  
H -3.9597519 -1.6780169 -1.6452535  
H -3.4414569 -2.7115595 -0.3014122  
H -3.8220204 -1.0051270 -0.0111144  
N 0.5417318 0.4801945 -0.6601626  
N 2.1073013 -0.0413091 0.7544865
```

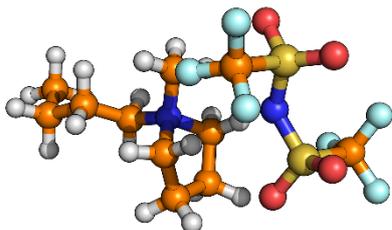


```
==> bmim_tfo_tpss_ontop.xyz <==  
E(TPSS-D3/def2-TZVP)= -1385.515676216  
C 1.6983035 -4.2946145 2.0136659  
F 0.9417707 -4.8062717 3.0149078  
F 2.6864496 -3.5602122 2.5843859  
F 2.2834525 -5.3331323 1.3705817  
O 0.1698777 -2.1865429 1.7202283  
O -0.3454308 -4.1939540 0.3595309  
O 1.6469668 -2.8225012 -0.1585281  
S 0.6631034 -3.2541750 0.8461769  
C -0.7013471 0.9315805 -1.7175795  
C 1.1037516 0.2109011 -0.1394813  
C -2.0709094 0.3132446 -1.4153729  
C -0.0253813 2.0031465 0.5003708  
C 0.8862201 1.7108242 1.4715237  
C -1.9847488 -1.1058261 -0.8430265  
C 2.6287006 -0.1153563 1.8025708  
C -3.3615987 -1.7313082 -0.5986486  
H 1.4246273 -0.6652875 -0.6827304  
H -0.7964392 1.9319784 -2.1448862  
H -0.1352384 0.3098290 -2.4151098  
H -0.7533297 2.7950632 0.4281333  
H 1.1053922 2.1991021 2.4073453  
H -2.6209596 0.9680983 -0.7272548  
H -2.6281509 0.3090930 -2.3605991  
H -1.4095365 -1.7405384 -1.5299810  
H -1.4270596 -1.0934517 0.0998471  
H 2.1900553 -0.5281233 2.7112914  
H 3.0022197 -0.9270987 1.1803712  
H 3.4297031 0.5855135 2.0413222  
H -3.9308727 -1.8157593 -1.5322259  
H -3.2560929 -2.7334756 -0.1707735  
H -3.9492844 -1.1238282 0.0998934  
N 0.1307490 1.0578627 -0.4999454  
N 1.5811382 0.5908535 1.0506790
```



```
==> bmpyr_ntf2_tpss_inplane.xyz <==  
E(TPSS-D3/def2-TZVP)= -2237.911009064  
C 0.1611188 -5.5219230 -2.3311563  
C -1.1792752 -2.8675946 -6.0374211  
F -0.9672660 -6.1682723 -2.6831570  
F 1.0940417 -5.7460924 -3.2713709  
F 0.6004048 -6.0352839 -1.1625721  
F -0.6833396 -2.3763192 -7.1917493  
F -1.4237537 -4.1794655 -6.2032282  
F -2.3401991 -2.2411215 -5.7726219  
N -0.7908354 -3.2133749 -3.4939249  
O -1.2040469 -3.6404951 -1.1000814  
O 1.1426938 -3.1188504 -1.8037230  
O 0.1974545 -1.1283090 -4.5770998  
O 1.2635654 -3.3260033 -5.0777001  
S -0.1664433 -3.6828203 -2.1154887  
S 0.0836606 -2.5761238 -4.6794470  
C 1.0405556 0.4231669 -1.8290427  
C -0.2939823 1.8045174 -0.4416938  
C 0.0704102 -0.5949342 0.2238337  
C 2.0334159 1.2959417 -1.0597976  
C 1.1549888 2.2377515 -0.1843098  
C -1.1391727 -0.8889421 1.1038052  
C -0.7096340 -1.6289736 2.3860586  
C -1.4157653 -0.0315721 -1.7139327  
C -0.0448289 -2.9894494 2.1326241  
H 1.3647839 -0.5954917 -2.0389234  
H 0.7178896 0.8935191 -2.7589069  
H -0.7509374 2.3707524 -1.2554173  
H -0.9494244 1.8362865 0.4278766  
H 0.4503519 -1.5053046 -0.2384490  
H 0.8746467 -0.1424358 0.8096359  
H 2.6921006 0.6865240 -0.4372153  
H 1.4130822 2.1423375 0.8724824  
H 1.2793069 3.2864270 -0.4599064  
H 2.6607317 1.8504330 -1.7597263  
H -1.6462518 0.0412450 1.3859095  
H -1.8542779 -1.5076756 0.5529429  
H -0.0315868 -0.9850799 2.9617801  
H -1.6044004 -1.7719606 3.0029571  
H -1.4780272 0.6103178 -2.5921684
```

H	-1.3175821	-1.0720432	-2.0184560
H	-2.2949904	0.1000815	-1.0850895
H	0.9057848	-2.8869318	1.5972653
H	-0.6912586	-3.6351290	1.5302388
H	0.1639122	-3.4945350	3.0815338
N	-0.1954483	0.3680970	-0.9357403

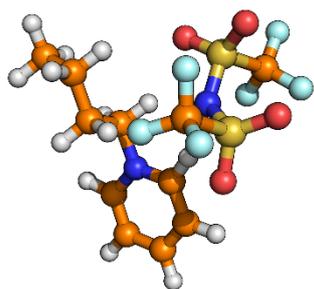


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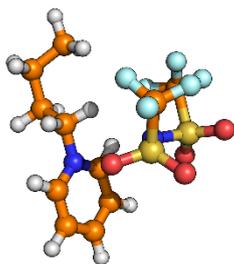
==> bmpyr_ntf2_tpss_ontop.xyz <==
E(TPSS-D3/def2-TZVP)= -2237.914422376
C  1.4658885  2.5735934 -5.9336089
C -2.3676109  4.6292497 -3.1481010
F  1.5780116  1.2830758 -5.5515394
F  0.5644222  2.6443208 -6.9298794
F  2.6605347  2.9817113 -6.4046373
F -3.6188572  5.0842752 -3.3528921
F -2.3354062  3.9929009 -1.9560788
F -1.5327590  5.6825287 -3.0877112
N -0.4276015  2.9764473 -4.0442114
O  1.9417134  3.3491038 -3.4603375
O  0.8918513  4.9988069 -5.0221221
O -1.9357889  4.2516147 -5.7426196
O -2.7887234  2.3354130 -4.3746023
S  0.9560191  3.6538288 -4.4828201
S -1.8763312  3.4553943 -4.5323935
C  0.7758403  0.0359106 -2.2934627
C  0.4714025  1.8339996 -0.7971996
C -0.0513336 -0.5165053 -0.0117908
C  2.1866165  0.4403840 -1.8471826
C  1.9785089  1.5824321 -0.8107025
C -0.8998168 -0.1660139  1.2067403
C -0.5949920 -1.1072628  2.3875235
C -1.5611446  0.6240720 -1.6310723
C -0.9505368 -2.5759321  2.1224548
H  0.6242552 -1.0305581 -2.4629786
H  0.4532608  0.5993239 -3.1710840
H  0.1722665  2.5116480 -1.5990866
H  0.0605294  2.1782023  0.1504791
H -0.3523884 -1.4717946 -0.4474271
H  1.0051152 -0.5811282  0.2584449
H  2.7206253 -0.4025092 -1.4035865
H  2.3371596  1.2863627  0.1779848
H  2.5004722  2.4943687 -1.1004595
H  2.7556243  0.7837948 -2.7120753
H -0.6992411  0.8637202  1.5207078
H -1.9646636 -0.2322046  0.9592103
H  0.4669101 -1.0206687  2.6525090
H -1.1633501 -0.7472738  3.2525639
H -1.5624751  1.2387048 -2.5289820
H -1.9506917 -0.3711095 -1.8486596

```

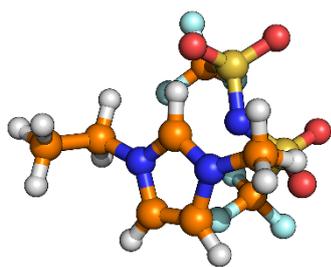
H	-2.1508145	1.0989951	-0.8478495
H	-0.3400116	-3.0076518	1.3215705
H	-2.0039867	-2.6755469	1.8347129
H	-0.7876736	-3.1793620	3.0211051
N	-0.1423340	0.4860734	-1.1595210



```
==> bpy_ntf2_tpss_inplane.xyz <==  
E(TPSS-D3/def2-TZVP)= -2234.297029608  
C -3.3045342 -4.1132628 -0.2669256  
C -1.2362084 -2.8149226 4.2877102  
F -4.4565983 -3.9160495 0.3992947  
F -3.0968921 -3.0523534 -1.0782804  
F -3.4325332 -5.2148074 -1.0318566  
F -1.6920911 -2.4842350 5.5125159  
F -0.8533593 -4.1044656 4.3054792  
F -0.1572302 -2.0536401 4.0149985  
N -1.8262988 -2.9039141 1.6513254  
O -2.1996744 -5.4772306 1.7284966  
O -0.7054856 -4.3932175 0.0364289  
O -2.7946372 -1.0981956 3.0198599  
O -3.6731143 -3.4091213 3.4190368  
S -1.8589052 -4.3249084 0.9170229  
S -2.5882671 -2.5370262 3.0117784  
C 0.4881501 -1.1583908 -0.5166172  
C 1.3900219 -1.2618487 0.7174384  
C -1.5352967 0.0071107 0.2379699  
C 0.0742940 1.2286758 -0.9774348  
C 2.2511591 -2.5349390 0.7034808  
C -2.3187370 1.1374336 0.3841386  
C -0.6776169 2.3832480 -0.8594014  
C -1.8913468 2.3426191 -0.1714795  
C 3.2652852 -2.5897879 -0.4465287  
H -0.1844737 -2.0158207 -0.5820815  
H 1.0570665 -1.0816205 -1.4440313  
H 1.0239826 1.1887381 -1.4960623  
H -1.7923917 -0.9616388 0.6528876  
H 2.0322643 -0.3729292 0.7686988  
H 0.7526603 -1.2618326 1.6083926  
H 2.7854578 -2.5806597 1.6599217  
H 1.5924306 -3.4099217 0.6659476  
H -0.3084088 3.2990103 -1.3049881  
H -3.2480984 1.0601087 0.9357325  
H -2.4929436 3.2392899 -0.0688749  
H 3.9004631 -3.4771886 -0.3581015  
H 3.9159252 -1.7070157 -0.4393669  
H 2.7724688 -2.6370434 -1.4242348  
N -0.3639386 0.0665061 -0.4382436
```



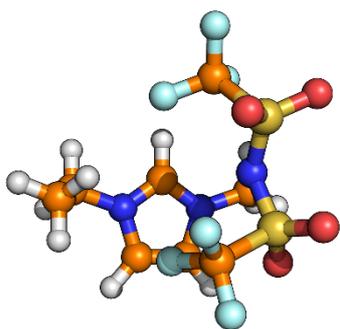
```
==> bpy_ntf2_tpss_ontop.xyz <==  
E(TPSS-D3/def2-TZVP)= -2234.297390117  
C -3.0007584 -1.8949653 -3.6719108  
C 0.9454514 -0.8368308 -4.5056684  
F -2.6780230 -2.1536193 -4.9514807  
F -2.2289611 -2.6615141 -2.8727901  
F -4.2894285 -2.2436063 -3.4769631  
F 1.8514164 -0.6795893 -5.4887747  
F 1.5979596 -0.8021035 -3.3200899  
F 0.3743597 -2.0467974 -4.6370055  
N -1.1998432 0.1554733 -3.3207590  
O -3.5548882 0.6347059 -4.2542338  
O -3.1683977 -0.0036173 -1.8627826  
O -0.9617534 0.3935094 -5.9017257  
O 0.4491509 1.7381102 -4.3321912  
S -2.7722483 -0.0742551 -3.2588737  
S -0.3293271 0.5404943 -4.6037063  
C -0.3252559 -0.6702500 -0.2116769  
C 0.9101817 -0.9742520 0.6393645  
C -1.6043656 1.3351989 0.4345178  
C 0.1751763 1.5597117 -1.0900727  
C 1.2014019 -2.4827832 0.7106941  
C -1.8735003 2.6891089 0.3572481  
C -0.0556134 2.9173898 -1.2030234  
C -1.0935367 3.4942280 -0.4729471  
C 1.6001989 -3.1066679 -0.6334236  
H -1.2221172 -1.1333760 0.2022548  
H -0.2125870 -0.9999110 -1.2457542  
H 0.9515360 1.0474320 -1.6409288  
H -2.1797276 0.6488406 1.0415938  
H 1.7784321 -0.4505290 0.2191211  
H 0.7480853 -0.5783260 1.6486153  
H 2.0130624 -2.6306348 1.4324582  
H 0.3241907 -3.0017838 1.1181525  
H 0.5646962 3.4991779 -1.8731193  
H -2.6939826 3.0961382 0.9355196  
H -1.2976281 4.5563379 -0.5554532  
H 1.8745297 -4.1584220 -0.5024159  
H 2.4601768 -2.5836598 -1.0670308  
H 0.7838198 -3.0692359 -1.3633830  
N -0.5915682 0.7950811 -0.2798114
```



==> emim_ntf2_tpss_inplane.xyz <==

E(TPSS-D3/def2-TZVP)= -2172.892799039

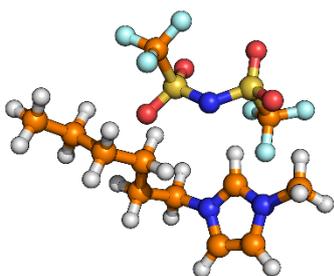
C	-0.9447965	-4.9530014	-2.2956782
C	2.1448766	-4.0996902	0.2409842
F	-0.0741245	-5.9703219	-2.1706748
F	-1.5016216	-4.7120204	-1.0909387
F	-1.9223255	-5.3311742	-3.1456436
F	3.3560246	-4.4873862	0.6924414
F	1.6435892	-3.1902617	1.0986135
F	1.3314785	-5.1715561	0.2358417
N	0.8410952	-2.9081990	-1.7760356
O	0.5758820	-3.8519607	-4.1683110
O	-1.1923970	-2.4595355	-3.0787090
O	2.8566828	-4.4747735	-2.2907915
O	3.1831197	-2.2144291	-1.2701307
S	-0.0958183	-3.4097338	-2.9603371
S	2.3417170	-3.3803262	-1.4864359
C	-0.2236194	-0.1287999	-1.2895691
C	-2.0678928	-1.1111709	0.0851850
C	0.2063332	-0.2586427	0.8752238
C	1.2977016	0.2794005	0.2622887
C	1.9284804	0.7890094	-2.1469695
C	-3.0678128	-0.0999201	0.6393814
H	-0.7104682	-0.2396840	-2.2440974
H	-2.3763608	-1.4987019	-0.8872605
H	-1.9335120	-1.9571407	0.7630531
H	0.0186582	-0.4880531	1.9114925
H	2.2468079	0.6011983	0.6581458
H	2.3534103	1.7558094	-1.8758600
H	1.3674358	0.8785495	-3.0764896
H	2.7139630	0.0389320	-2.2500453
H	-3.1936434	0.7389343	-0.0512100
H	-4.0360388	-0.5913822	0.7720827
H	-2.7409616	0.2860733	1.6094329
N	-0.7310132	-0.5097997	-0.1118523
N	1.0052364	0.3583104	-1.0881505



```

==> emim_ntf2_tpss_ontop.xyz <==
E(TPSS-D3/def2-TZVP)= -2172.890107569
C -2.0887935 3.7684231 -0.2818376
C -1.3841266 0.8000035 -4.0368479
F -3.2546245 3.8302893 -0.9476172
F -2.0370241 2.5908466 0.3757353
F -2.0657034 4.7637313 0.6313138
F -1.9601541 0.5202277 -5.2199379
F -0.1299597 0.2971548 -4.0462924
F -2.0801985 0.1745135 -3.0649648
N -0.6872486 2.6531832 -2.3550033
O -0.8574370 5.2133725 -2.1294790
O 0.5213535 3.8417711 -0.5486461
O -2.7825735 3.0455453 -3.8279204
O -0.5159637 3.1639867 -4.8592649
S -0.6184555 3.9532434 -1.4435023
S -1.3800303 2.6633612 -3.8020039
C 0.2762022 -0.3374741 -0.8021771
C -1.6157488 -1.4701234 0.3859357
C 0.0234865 0.2580018 1.3120573
C 1.0644532 0.9698244 0.7955119
C 2.2011275 1.1055952 -1.4723820
C -2.9361380 -0.7060796 0.4448784
H 0.1420759 -0.8289785 -1.7511806
H -1.5653617 -2.1163591 -0.4922483
H -1.4680750 -2.0880164 1.2742036
H -0.4156133 0.2609747 2.2962604
H 1.6997463 1.7183519 1.2385498
H 2.0719699 2.1850360 -1.5421404
H 2.0253410 0.6454984 -2.4430804
H 3.2007933 0.8565068 -1.1137455
H -3.0668107 -0.0826176 -0.4434507
H -3.7577939 -1.4263596 0.4938051
H -2.9842366 -0.0685041 1.3320902
N -0.4553076 -0.5545148 0.2981016
N 1.2073908 0.5814811 -0.5238697

```

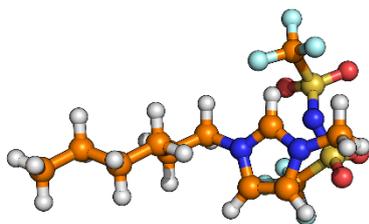


```

==> hmim_ntf2_tpss_inplane.xyz <==
E(TPSS-D3/def2-TZVP)= -2330.237178673
C  0.7330626  2.8582303 -4.0886577
C  2.5371125  5.1514735  0.1411406
F -0.2451426  2.0145141 -3.7042678
F  0.1897546  4.0722935 -4.2852226
F  1.2387102  2.4193232 -5.2592178
F  2.3821859  6.3423507  0.7522014
F  2.6483440  4.1976116  1.0930294
F  3.6780653  5.1763771 -0.5667260
N  1.3208309  3.3194199 -1.4655382
O  2.5388270  1.5488048 -2.6750602
O  3.0419223  3.9149134 -3.3231924
O  1.0666862  5.8712003 -1.9502510
O -0.0566283  4.7459638 -0.0134688
S  2.1103978  2.9295383 -2.8065304
S  1.0490238  4.8122064 -0.9599067
C  2.0202437  0.3136168  0.4428317
C  0.4053124  1.8932886  1.5144751
C  1.2966414 -0.7520674 -0.3839136
C -0.0161641 -0.2514450 -0.9979090
C  1.0635657  0.2281017  2.8144877
C -0.6605657 -1.2463525 -1.9756532
C  0.1803611  0.9887503  3.5229680
C  0.1743509 -1.5265784 -3.2333731
C -1.1516465  3.1057491  3.0396149
C -0.5734879 -2.4052584 -4.2431895
H  0.2949183  2.5515564  0.6663874
H  2.2547471  1.1798462 -0.1774164
H  2.9438487 -0.0722420  0.8778356
H  1.6119234 -0.6588554  3.0881675
H -0.1882250  0.8931070  4.5314605
H  1.9986418 -1.0373242 -1.1746232
H  1.1184065 -1.6453108  0.2281075
H -0.7336434 -0.0347492 -0.1953925
H  0.1741541  0.6943609 -1.5184450
H -0.8638186 -2.1937897 -1.4557570
H -1.6361740 -0.8461022 -2.2831855
H  1.1159725 -2.0171447 -2.9559657
H  0.4492278 -0.5731609 -3.7014041
H -2.1511234  2.6889339  3.1709309
H -1.1500512  3.8307542  2.2260398

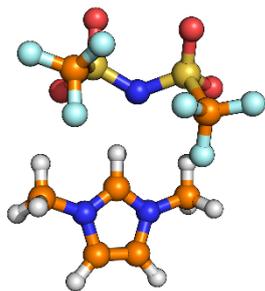
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H	-0.8179295	3.5791141	3.9637224
H	-0.8518778	-3.3673439	-3.7957742
H	-1.4950869	-1.9151547	-4.5801349
H	0.0416344	-2.6105642	-5.1263540
N	1.1956522	0.8134094	1.5675610
N	-0.2158252	2.0245622	2.6939060



```
==> hmim_ntf2_tpss_ontop.xyz <==  
E(TPSS-D3/def2-TZVP)= -2330.230753835  
C 4.2739269 3.0705113 1.4362799  
C 2.8294275 -0.4010766 4.8269044  
F 3.9689631 2.0485954 0.6060727  
F 3.2756314 3.9755835 1.3722405  
F 5.4044437 3.6502357 0.9949727  
F 2.2512326 -0.9612539 5.9102119  
F 2.3045359 -0.9791546 3.7245131  
F 4.1459640 -0.6730776 4.8588502  
N 3.0615908 1.9348296 3.4236393  
O 5.5565001 1.4140011 3.0538526  
O 4.9159059 3.6506101 3.9472336  
O 3.2599794 1.9256149 5.9959228  
O 1.0687823 1.5539428 4.8382239  
S 4.5578975 2.4622516 3.1901473  
S 2.5177318 1.4560808 4.8370542  
C 1.8055559 -0.5803249 0.2729901  
C 0.7657691 1.5163406 1.1630570  
C 1.1641152 -1.6974264 -0.5489342  
C 0.1399235 -1.2009350 -1.5777156  
C -0.1812563 -0.3502912 1.8728356  
C -0.5477048 -2.3396016 -2.3480604  
C -0.8257724 0.6974113 2.4577817  
C 0.3880543 -3.1475827 -3.2589498  
C -0.5336598 3.2202711 2.4380748  
C -0.3546256 -4.2443881 -4.0315980  
H 1.4165300 2.2050520 0.6520755  
H 2.3026076 0.1464660 -0.3729325  
H 2.5417748 -0.9779374 0.9769089  
H -0.3369613 -1.4118159 1.9669342  
H -1.6420333 0.7225547 3.1606641  
H 1.9889886 -2.2193275 -1.0456385  
H 0.6988386 -2.4309293 0.1223123  
H -0.6294707 -0.6081045 -1.0655258  
H 0.6386092 -0.5238825 -2.2853349  
H -1.0307187 -3.0189991 -1.6304772  
H -1.3535656 -1.9132490 -2.9603314  
H 1.1879289 -3.6059359 -2.6636732  
H 0.8787942 -2.4640089 -3.9657319  
H -1.5981725 3.4067912 2.2937353  
H 0.0502994 3.9167469 1.8376025
```

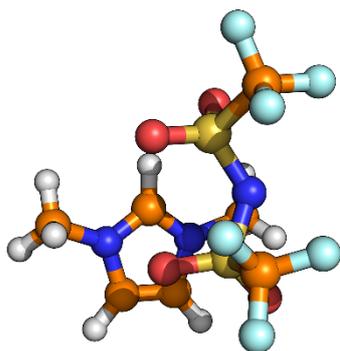
H	-0.2650222	3.3136656	3.4911895
H	-0.8191644	-4.9605836	-3.3429115
H	-1.1500759	-3.8152393	-4.6528673
H	0.3239902	-4.8004024	-4.6879452
N	0.8105193	0.1819085	1.0656231
N	-0.2212383	1.8531342	1.9998218



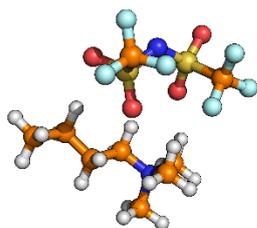
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==> mmim_ntf2_tpss_inplane.xyz <==
E(TPSS-D3/def2-TZVP)= -2133.552967011
C  0.2799477 -1.5175743 -5.2773034
C  3.7396763 -1.1490213 -3.1406109
F  0.2334748 -0.3233160 -4.6470616
F  1.3735078 -1.5491797 -6.0567604
F -0.8098254 -1.6226056 -6.0634563
F  5.0838412 -1.2395334 -3.1255081
F  3.3686454 -0.4714095 -4.2404218
F  3.3499978 -0.4427174 -2.0568473
N  1.4485637 -2.5379049 -2.9921701
O -0.9679830 -2.7358802 -3.3170969
O  0.4999850 -4.1214865 -4.8043125
O  3.4718906 -3.4118323 -1.8395893
O  3.4500405 -3.5055227 -4.3444072
S  0.2927095 -2.9194698 -4.0212696
S  3.0078686 -2.8828398 -3.1108045
C  0.2447607 -0.6881760 -0.6964116
C  0.5400025  0.7253572  0.9823201
C -0.5155235  1.1678201  0.2414606
C -1.6919569  0.3632704 -1.8681791
C  2.1273128 -1.2596484  0.8384508
H  0.3886718 -1.5139176 -1.3805887
H -1.1537105  2.0282897  0.3614369
H  0.9970051  1.1247187  1.8732719
H -1.4565583  1.2122626 -2.5119278
H -1.6664598 -0.5630658 -2.4403898
H  1.9006669 -1.6502322  1.8314030
H  2.2642678 -2.0789082  0.1338740
H  3.0273654 -0.6445663  0.8715785
H -2.6738873  0.4967136 -1.4133174
N  1.0002793 -0.4327433  0.3791759
N -0.6830623  0.2717553 -0.8006042

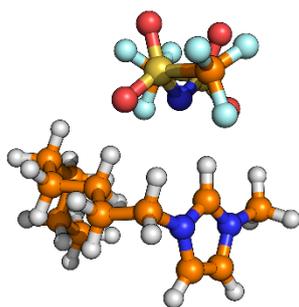
```



```
==> mmim_ntf2_tpss_ontop.xyz <==  
E(TPSS-D3/def2-TZVP)= -2133.554071727  
C 0.4729333 5.2515491 -1.0617952  
C 2.7718540 3.2161635 -3.7757509  
F 1.7069118 5.7850467 -0.9776643  
F 0.0286506 5.3891117 -2.3248169  
F -0.3472460 5.9468606 -0.2463755  
F 2.9411430 2.6808812 -5.0021040  
F 2.2395146 4.4432563 -3.9168930  
F 3.9782255 3.3375400 -3.1926054  
N 1.7012799 2.7892365 -1.3379499  
O 0.8605145 3.4913505 0.8575420  
O -0.8439683 2.9652514 -0.8973964  
O 2.3852826 0.8424804 -2.7206960  
O 0.3680551 2.1078731 -3.4718650  
S 0.4816575 3.4419015 -0.5434401  
S 1.6428495 2.0948032 -2.7744767  
C 0.1223086 -0.1782369 -0.6215338  
C -0.3035981 0.3504495 1.4835078  
C -1.4929801 0.2542215 0.8247392  
C -2.1712595 -0.1437945 -1.5912286  
C 2.1397209 0.1217993 0.8171351  
H 0.6514324 -0.4138130 -1.5308692  
H -2.5043576 0.4039164 1.1652616  
H -0.0793337 0.5951696 2.5086883  
H -1.7300385 -0.7155088 -2.4068315  
H -3.0759046 -0.6373196 -1.2372749  
H 2.4009066 -0.6481231 1.5442295  
H 2.6567242 -0.0510571 -0.1253583  
H 2.3906102 1.1128362 1.1968857  
H -2.3921211 0.8729417 -1.9211325  
N 0.6920696 0.0786117 0.5626123  
N -1.2051908 -0.0789552 -0.4860164
```



```
==> n1114_ntf2_tpss_inplane.xyz <==  
E(TPSS-D3/def2-TZVP)= -2160.448195877  
C 5.1555314 -0.2635567 2.9002779  
C 4.0221423 3.6084989 1.8400548  
F 5.8470912 0.6417296 2.1825324  
F 5.6712981 -0.3106849 4.1424904  
F 5.3151702 -1.4741626 2.3264245  
F 3.6064846 4.8155042 1.4010123  
F 5.2277936 3.7570182 2.4183015  
F 4.1585544 2.7981354 0.7712168  
N 3.3936940 1.5889623 3.6426662  
O 2.9153491 0.1346216 1.5383330  
O 2.7568003 -0.8276017 3.8413501  
O 1.5563417 2.7652009 2.2681501  
O 2.7642075 3.9155194 4.1314452  
S 3.3235326 0.1533230 2.9334285  
S 2.7639188 2.9279659 3.0679153  
C -0.3107415 0.4435590 0.5680149  
C 0.1181183 -1.0059510 0.3866233  
C -0.0814649 -1.7689603 1.7075167  
C -0.6342724 2.7187286 -0.3067981  
C -0.8382164 0.8244383 -1.8528021  
C 1.3704793 1.4765324 -0.9725180  
C 0.4594984 -3.1994996 1.6261490  
H -1.3782860 0.5136355 0.7942811  
H 0.2583265 0.9165062 1.3711645  
H -0.4641847 -1.4930972 -0.4035448  
H 1.1762196 -1.0555319 0.1130755  
H 0.4357330 -1.2338349 2.5121277  
H -1.1491908 -1.7839417 1.9618476  
H -0.7357068 1.5520989 -2.6583772  
H -1.6973689 2.6251927 -0.0842113  
H -0.0891653 3.0889281 0.5612436  
H -1.8875129 0.6983471 -1.5839153  
H -0.4011095 -0.1270273 -2.1505237  
H -0.4813111 3.3718519 -1.1666761  
H 1.4735390 2.1896249 -1.7910040  
H 1.8827767 1.8226419 -0.0765434  
H 1.7512522 0.5023449 -1.2730322  
H 0.3049432 -3.7314937 2.5707017  
H -0.0378045 -3.7671570 0.8308945  
H 1.5350286 -3.1908084 1.4159049  
N -0.0982191 1.3494873 -0.6514722
```

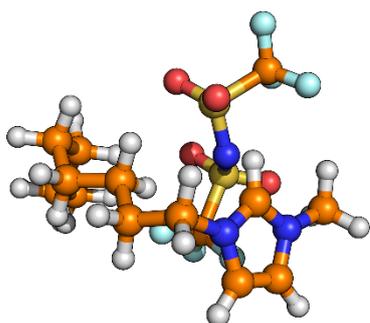


```

==> omim_ntf2_tpss_inplane.xyz <==
E(TPSS-D3/def2-TZVP)= -2408.909544038
C  5.2055647 -2.6155602 -2.0502857
C  3.4134705  2.1888015 -2.5996349
F  4.1039223 -3.3931972 -1.9621555
F  5.5210342 -2.4740790 -3.3499356
F  6.2200597 -3.2447643 -1.4266884
F  3.5209885  3.1071506 -3.5802814
F  2.2160043  2.3379580 -2.0033872
F  4.3764374  2.4203870 -1.6886005
N  3.5827627 -0.4585738 -2.0210407
O  4.5094116 -1.2856056  0.1150266
O  6.1104848 -0.1847441 -1.4624674
O  4.7954669  0.5013328 -4.1179024
O  2.3091593  0.2428001 -4.0049461
S  4.8963621 -0.9465115 -1.2427607
S  3.5792969  0.4617396 -3.3293700
C  1.3240957 -2.4440257  0.4042799
C  0.5617814 -1.7546549 -1.8768900
C  1.1542218 -1.3599144  1.4731100
C  1.2399741  0.0637728  0.9118093
C  1.2924631  1.1268550  2.0163019
C  1.3890372  2.5673193  1.4827827
C  0.1923414  3.0337155  0.6354919
C -1.0130153 -2.6519643 -0.6054585
C -1.5842646 -2.2954915 -1.7913601
C -1.1493943  3.0368013  1.3814251
C -0.7448440 -1.2398706 -3.9463661
C -2.2937445  3.5928708  0.5260740
H  1.2108573 -3.4466150  0.8220499
H  2.3059419 -2.3642108 -0.0644651
H  1.5173184 -1.3689383 -2.2057699
H  0.2037284 -1.5048596  2.0029750
H  1.9546707 -1.5239553  2.2046880
H -1.4346633 -3.1172848  0.2712589
H -2.5952650 -2.3963696 -2.1508627
H  2.1323994  0.1497926  0.2783888
H  0.3741426  0.2492951  0.2630536
H  0.4102390  1.0246725  2.6629715
H  2.1656158  0.9278720  2.6520831
H  1.5046116  3.2499561  2.3355968

```

H	2.3045912	2.6585477	0.8827697
H	0.1035991	2.4088966	-0.2626875
H	0.3977377	4.0515789	0.2750601
H	-1.0513290	3.6327669	2.2996063
H	-1.4003156	2.0164653	1.7007721
H	-0.9876503	-2.0782832	-4.6009545
H	0.1923880	-0.7789610	-4.2530077
H	-1.5504091	-0.5045611	-3.9660556
H	-2.4288970	2.9926542	-0.3824533
H	-2.0850012	4.6238766	0.2152119
H	-3.2428770	3.5905517	1.0739031
N	0.3257819	-2.3121139	-0.6816515
N	-0.5855870	-1.7362465	-2.5696113



```

==> omim_ntf2_tpss_ontop.xyz <==
E(TPSS-D3/def2-TZVP)= -2408.908533737
C  1.0629805  1.6714038 -4.3204171
C -2.9129119  0.4680179 -1.1675155
F  1.1406999  0.4341736 -4.8550021
F  0.0388909  2.3228005 -4.9068337
F  2.2049713  2.3277833 -4.6047021
F -4.1792134  0.9280091 -1.1224936
F -2.9558693 -0.8621262 -1.3923653
F -2.3420160  0.6734798  0.0309740
N -0.5378216  0.7731528 -2.2987629
O  1.9044458  0.7267749 -2.0094887
O  0.8107325  2.9743403 -2.0392173
O -2.1973327  2.7749788 -2.2947972
O -2.5984756  0.7908191 -3.7589418
S  0.8187459  1.5871681 -2.4565201
S -2.0073264  1.3604867 -2.5578300
C  1.5523447 -2.2095020  0.9171105
C  0.6036712 -2.0755253 -1.4035104
C  1.0597576 -1.1574440  1.9144120
C  0.9771786  0.2679171  1.3525385
C  0.7506634  1.3002237  2.4669395
C  0.7820319  2.7635748  1.9902903
C -0.4475290  3.2326446  1.1961723
C -0.5264688 -3.3637061 -0.0021516
C -1.1473201 -3.4163827 -1.2139117
C -1.7423294  3.2822134  2.0188421
C -0.7511546 -2.3402360 -3.4830590
C -2.9054156  3.9150462  1.2451844
H  1.7709796 -3.1544505  1.4195569
H  2.4590997 -1.8737823  0.4090919
H  1.3264149 -1.3786399 -1.8009235
H  0.0927089 -1.4691941  2.3287829
H  1.7755761 -1.1764404  2.7463358
H -0.7516711 -3.8549957  0.9305196
H -2.0232307 -3.9543646 -1.5380212
H  1.9154480  0.5030627  0.8327538
H  0.1838854  0.3333160  0.5990861
H -0.1992487  1.0889117  2.9766371
H  1.5378431  1.1625547  3.2212728
H  0.8960314  3.4141401  2.8688464

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H	1.6809468	2.9100101	1.3754733
H	-0.5966210	2.5997224	0.3156024
H	-0.2419232	4.2381729	0.8043734
H	-1.5625294	3.8524435	2.9420220
H	-2.0251600	2.2688847	2.3313071
H	-0.9276302	-3.2909249	-3.9872612
H	0.0922196	-1.8254555	-3.9390666
H	-1.6377481	-1.7075852	-3.5340554
H	-3.0983273	3.3720280	0.3139815
H	-2.6738648	4.9533931	0.9779698
H	-3.8273384	3.9164212	1.8383541
N	0.5671109	-2.5249726	-0.1426308
N	-0.4250250	-2.6080526	-2.0746437