7 Electronic Supplementary Information (SI)

7.1 SI–Potential Energy Surfaces

Presented here are five additional potential energy surfaces/curves referred to in the paper. None present new qualitative behavior, but they do confirm and/or rule out the possibility of conjectured structures.
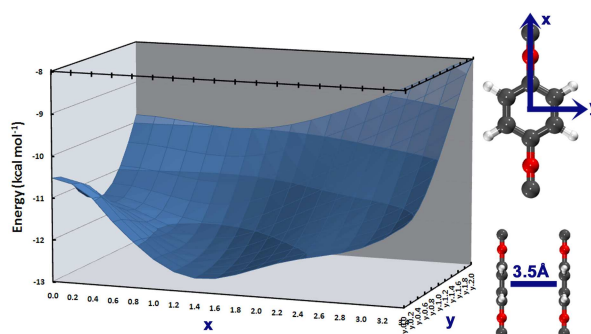

Figure 10: Two-dimensional potential energy surface for PDI dimer. Two frozen monomers (aug-cc-pVDZ geometry) were fixed at a vertical face-to-face distance of 3.5Å. The "upper" monomer was displaced along the isocyano axis (x), as well as the perpendicular in-plane axis (y). Energies are non-counterpoise-corrected aug-cc-pVDZ single points.
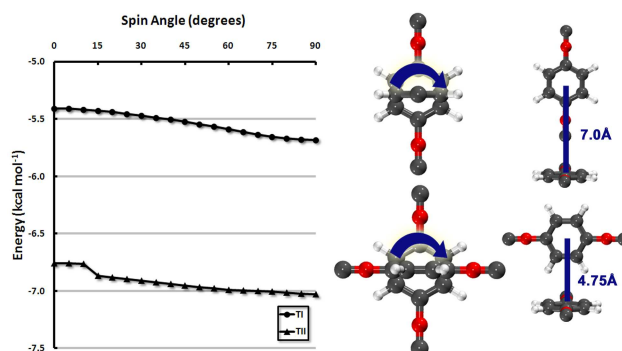
Figure 11: T-shaped rotational potential energy scans, in which one monomer was rotated relative to the other. The 0° and 90° endpoints correspond to analogues of the **TI-0** and **TI-90** (**TII-0** and **TII-90**) structures. Frozen monomers (aug-cc-pVDZ geometry) are employed. The TI center-to-center distance was fixed at 7.0 Å, and the TII center-to-center distance was fixed at 4.75 Å. Energies are non-counterpoise-corrected aug-cc-pVDZ single points. The discontinuity at 15° for TII is the point at which linear dependence in the AO basis vanishes. The same artifact is found in single-basis results.
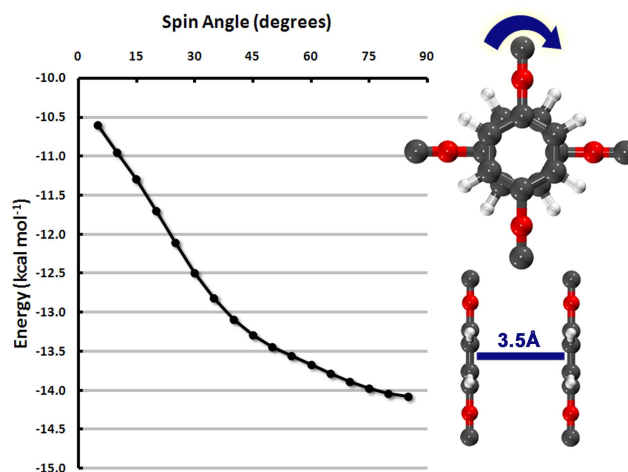
Figure 12: Parallel-displaced rotational potential energy scans, in which one monomer was rotated relative to the other. The 0° endpoint corresponds to an analogue of the sandwich (**S**) structure; the 90° endpoint corresponds to an analogue of the rotated-parallel (**RP-0**) structure. Frozen monomers (aug-cc-pVDZ geometry) are employed. The center-to-center distance was fixed at 3.5 Å, and energies are non-counterpoise-corrected aug-cc-pVDZ single points.

7.2   SI–PDI Surface Models

	Basis Set	I_1	I_2	I_3	Total
Non-CP	aug-cc-pVDZ	-2.59	-4.21	0.23	-10.79
	aug-cc-pVTZ	-1.59	-2.72	0.40	-6.64
	aug-cc-pVQZ	-1.18	-1.91	0.51	-4.49
	T→Q	-1.00	-1.48	0.57	-3.38
CP	aug-cc-pVDZ	-0.91	-0.73	0.55	-1.83
	aug-cc-pVTZ	-0.96	-1.19	0.54	-2.81
	aug-cc-pVQZ	-0.97	-1.36	0.54	-3.15
	T→Q	-0.97	-1.46	0.54	-3.35

Table 3: Basis set dependence of $\Theta = 1$ (Standard) surface configuration model. Refer to text, section 3.3, for details of models. All I_n's are dimer interaction energies in kcal mol^{-1}. The "Total" column is listed in kcal mol^{-1} monomer^{-1}

	Basis Set	I_1	I_2	Total
Non-CP	aug-cc-pVDZ	-3.32	-5.11	-13.53
	aug-cc-pVTZ	-2.38	-3.24	-8.85
	aug-cc-pVQZ	-1.84	-2.30	-6.45
	T→Q	-1.57	-1.82	-5.21
CP	aug-cc-pVDZ	-1.50	-2.54	-6.58
	aug-cc-pVTZ	-1.56	-1.99	-5.53
	aug-cc-pVQZ	-1.58	-1.92	-5.42
	T→Q	-1.59	-1.93	-5.45

Table 4: Basis set dependence of $\Theta = 1$ (Herringbone) surface configuration model. Refer to text, section 3.3, for details of models. All I_n's are dimer interaction energies in kcal mol^{-1}. The "Total" column is listed in kcal mol^{-1} monomer^{-1}

	Basis Set	I_1	I_2	Total
Non-CP	aug-cc-pVDZ	0.04	0.05	0.15
	aug-cc-pVTZ	0.07	0.14	0.35
	aug-cc-pVQZ	0.09	0.18	0.45
	T→Q	0.10	0.20	0.49
CP	aug-cc-pVDZ	0.10	0.22	0.54
	aug-cc-pVTZ	0.10	0.21	0.52
	aug-cc-pVQZ	0.10	0.21	0.52
	T→Q	0.10	0.21	0.52

Table 5: Basis set dependence of $\Theta = \frac{1}{3}$ (Standard) surface configuration model. Refer to text, section 3.3, for details of models. All I_n's are dimer interaction energies in kcal mol^{-1}. The "Total" column is listed in kcal mol^{-1} monomer^{-1}

Configuration	Model	I_1	I_2	I_3	I_4	2-body Total	Periodic Total	Periodic +D Total
$\Theta = 1$ Standard	$I_1 + 2I_2 + I_3 + 2I_4$	0.87	3.41	0.75	0.23	8.90	8.86	2.08
$\Theta = 1$ Herringbone	$I_1 + 2I_2 + I_3 + 2I_4$	1.30	1.31	0.25	0.36	4.89	5.04	-0.46
$\Theta = \frac{1}{3}$ Standard	$I_1 + 2I_2$	0.22	0.38			0.98	1.07	0.92

Table 6: Cohesive energies of PDI monolayers, calculated using the plane-wave protocol of Ref. [60]. Shown are the constituent energies and resulting monolayer energies, using (1) the plane-wave protocol for the calculation of dimer interaction energies in the two-body models, (2) the full periodic plane wave results of Li, and (3) the periodic results, including the empirical PBE-D term. Note that the remaining next-nearest-neighbor interaction (excluded in table 2) is also included for completeness. Note also that the PBE-optimized 40.9° rotation angle has been utilized for the Herringbone structure. The I_3 and I_4 interaction energies for the Herringbone structure (not shown in Fig. 7 of the text) are, respecitvely, the dimer connecting the short diagonal of the parallelogram in Fig. 7 and the dimer connecting the endpoints of the I_1/I_2 arrows in the same figure.

7.3 SI–Cartesian Coordinates of PDI Dimer Structures

This section contains cartesian coordinates of all of the 1,4-phenylenediisocyanide dimer optimized structures presented in the paper. The structures are DB-RI-MP2 structures using the dual-basis pairings for aug-cc-pVDZ and aug-cc-pVTZ.

Sandwich (**S**)

aug-cc-pVDZ:
```
c  1.39237498 -1.70694932  0.00000000
c -1.39237498 -1.70694932  0.00000000
c  0.70085833 -1.70778936 -1.22836877
c  0.70085833 -1.70778936  1.22836877
c -0.70085833 -1.70778936  1.22836877
c -0.70085833 -1.70778936 -1.22836877
h  1.26543571 -1.71834339 -2.16411873
h  1.26543571 -1.71834339  2.16411873
h -1.26543571 -1.71834339  2.16411873
h -1.26543571 -1.71834339 -2.16411873
n  2.78289400 -1.73232532  0.00000000
n -2.78289400 -1.73232532  0.00000000
c  3.98289420 -1.78345306  0.00000000
c -3.98289420 -1.78345306  0.00000000
c  1.39237498  1.70694932  0.00000000
c -1.39237498  1.70694932  0.00000000
c  0.70085833  1.70778936 -1.22836877
c  0.70085833  1.70778936  1.22836877
c -0.70085833  1.70778936  1.22836877
c -0.70085833  1.70778936 -1.22836877
h  1.26543571  1.71834339 -2.16411873
h  1.26543571  1.71834339  2.16411873
h -1.26543571  1.71834339  2.16411873
h -1.26543571  1.71834339 -2.16411873
n  2.78289400  1.73232532  0.00000000
n -2.78289400  1.73232532  0.00000000
c  3.98289420  1.78345306  0.00000000
c -3.98289420  1.78345306  0.00000000
```

aug-cc-pVTZ:
```
c  1.38052397 -1.74966556  0.00000000
c -1.38052397 -1.74966556  0.00000000
c  0.69418353 -1.74872528 -1.21647338
c  0.69418353 -1.74872528  1.21647338
c -0.69418353 -1.74872528  1.21647338
c -0.69418353 -1.74872528 -1.21647338
h  1.25244588 -1.75548986 -2.14270931
h  1.25244588 -1.75548986  2.14270931
h -1.25244588 -1.75548986  2.14270931
h -1.25244588 -1.75548986 -2.14270931
n  2.76045555 -1.76619239  0.00000000
n -2.76045555 -1.76619239  0.00000000
c  3.94598779 -1.81054996  0.00000000
c -3.94598779 -1.81054996  0.00000000
c  1.38052397  1.74966556  0.00000000
c -1.38052397  1.74966556  0.00000000
c  0.69418353  1.74872528 -1.21647338
c  0.69418353  1.74872528  1.21647338
c -0.69418353  1.74872528  1.21647338
c -0.69418353  1.74872528 -1.21647338
h  1.25244588  1.75548986 -2.14270931
h  1.25244588  1.75548986  2.14270931
h -1.25244588  1.75548986  2.14270931
h -1.25244588  1.75548986 -2.14270931
n  2.76045555  1.76619239  0.00000000
n -2.76045555  1.76619239  0.00000000
c  3.94598779  1.81054996  0.00000000
c -3.94598779  1.81054996  0.00000000
```

Parallel Displaced (**PD-0**)

aug-cc-pVDZ:
```
c  0.21207966 -1.69883266  1.39179723
c  0.21207966 -1.69883266 -1.39179723
c  1.26063307 -1.05623408  0.70094006
c -0.83636442 -2.33901764  0.70103682
c -0.83636442 -2.33901764 -0.70103682
c  1.26063307 -1.05623408 -0.70094006
h  2.06529536 -0.57872477  1.26570922
h -1.62972654 -2.83521440  1.26551880
h -1.62972654 -2.83521440 -1.26551880
h  2.06529536 -0.57872477 -1.26570922
n  0.21996208 -1.71791214  2.78226277
n  0.21996208 -1.71791214 -2.78226277
c  0.22365092 -1.76403846  3.98261059
c  0.22365092 -1.76403846 -3.98261059
c -0.21207966  1.69883266  1.39179723
c -0.21207966  1.69883266 -1.39179723
c  0.83636442  2.33901764  0.70103682
c -1.26063307  1.05623408  0.70094006
c -1.26063307  1.05623408 -0.70094006
c  0.83636442  2.33901764 -0.70103682
h  1.62972654  2.83521440  1.26551880
h -2.06529536  0.57872477  1.26570922
h -2.06529536  0.57872477 -1.26570922
h  1.62972654  2.83521440 -1.26551880
n -0.21996208  1.71791214  2.78226277
n -0.21996208  1.71791214 -2.78226277
c -0.22365092  1.76403846  3.98261059
c -0.22365092  1.76403846 -3.98261059
```

aug-cc-pVTZ:
```
c  0.20584739 -1.73064133  1.38022842
c  0.20584739 -1.73064133 -1.38022842
c  1.25077331 -1.10579174  0.69427278
c -0.84007363 -2.35183404  0.69423650
c -0.84007363 -2.35183404 -0.69423650
c  1.25077331 -1.10579174 -0.69427278
h  2.05012369 -0.63781116  1.25299448
h -1.63205150 -2.83213906  1.25258359
h -1.63205150 -2.83213906 -1.25258359
h  2.05012369 -0.63781116 -1.25299448
n  0.20865182 -1.74300817  2.75992605
n  0.20865182 -1.74300817 -2.75992605
c  0.20605537 -1.78598749  3.94565649
c  0.20605537 -1.78598749 -3.94565649
c -0.20584739  1.73064133  1.38022842
c -0.20584739  1.73064133 -1.38022842
c  0.84007363  2.35183404  0.69423650
c -1.25077331  1.10579174  0.69427278
c -1.25077331  1.10579174 -0.69427278
c  0.84007363  2.35183404 -0.69423650
h  1.63205150  2.83213906  1.25258359
h -2.05012369  0.63781116  1.25299448
h -2.05012369  0.63781116 -1.25299448
h  1.63205150  2.83213906 -1.25258359
n -0.20865182  1.74300817  2.75992605
n -0.20865182  1.74300817 -2.75992605
c -0.20605537  1.78598749  3.94565649
c -0.20605537  1.78598749 -3.94565649
```

7.3 SI–Cartesian Coordinates of PDI Dimer Structures

Parallel Displaced (**PD-90C**)

aug-cc-pVDZ:
c 0.14037700 -1.70838314 0.00000000
c -2.50668270 -0.83703593 0.00000000
c -0.51656375 -1.48996261 -1.22803447
c -0.51656375 -1.48996261 1.22803447
c -1.84867093 -1.05180939 1.22825280
c -1.84867093 -1.05180939 -1.22825280
h 0.01510632 -1.68017134 -2.16379148
h 0.01510632 -1.68017134 2.16379148
h -2.38848417 -0.88470929 2.16361083
h -2.38848417 -0.88470929 -2.16361083
n 1.45043856 -2.17564489 0.00000000
n -3.83636755 -0.43598882 0.00000000
c 2.56624185 -2.62106624 0.00000000
c -4.98805495 -0.09675532 0.00000000
c 2.50668270 0.83703593 0.00000000
c -0.14037700 1.70838314 0.00000000
c 1.84867093 1.05180939 -1.22825280
c 1.84867093 1.05180939 1.22825280
c 0.51656375 1.48996261 1.22803447
c 0.51656375 1.48996261 -1.22803447
h 2.38848417 0.88470929 -2.16361083
h 2.38848417 0.88470929 2.16361083
h -0.01510632 1.68017134 2.16379148
h -0.01510632 1.68017134 -2.16379148
n 3.83636755 0.43598882 0.00000000
n -1.45043856 2.17564489 0.00000000
c 4.98805495 0.09675532 0.00000000
c -2.56624185 2.62106624 0.00000000

aug-cc-pVTZ:
C 0.05819700 -1.73593500 0.00000000
C -2.54303000 -0.80576000 0.00000000
C -0.58707700 -1.50070000 -1.21626800
C -0.58707700 -1.50070000 1.21626800
C -1.89480600 -1.03308300 1.21635700
C -1.89480600 -1.03308300 -1.21635700
H -0.06377200 -1.69520600 -2.14262000
H -0.06377200 -1.69520600 2.14262000
H -2.42245600 -0.84989500 2.14241400
H -2.42245600 -0.84989500 -2.14241400
N 1.35138300 -2.21843700 0.00000000
N -3.84960400 -0.36776500 0.00000000
C 2.44961000 -2.66820800 0.00000000
C -4.97929800 -0.00694900 0.00000000
C 2.54303000 0.80576000 0.00000000
C -0.05819700 1.73593500 0.00000000
C 1.89480600 1.03308300 -1.21635700
C 1.89480600 1.03308300 1.21635700
C 0.58707700 1.50070000 1.21626800
C 0.58707700 1.50070000 -1.21626800
H 2.42245600 0.84989500 -2.14241400
H 2.42245600 0.84989500 2.14241400
H 0.06377200 1.69520600 2.14262000
H 0.06377200 1.69520600 -2.14262000
N 3.84960400 0.36776500 0.00000000
N -1.35138300 2.21843700 0.00000000
C 4.97929800 0.00694900 0.00000000
C -2.44961000 2.66820800 0.00000000

Parallel Displaced (**PD-90N**)

aug-cc-pVDZ:
c -0.69904423 -1.39141245 0.00000000
c -3.29036523 -0.37909604 0.00000000
c -1.34253555 -1.14290237 -1.22908024
c -1.34253555 -1.14290237 1.22908024
c -2.64840286 -0.63325866 1.22864594
c -2.64840286 -0.63325866 -1.22864594
h -0.81899680 -1.35630199 -2.16447236
h -0.81899680 -1.35630199 2.16447236
h -3.17365214 -0.42434486 2.16354639
h -3.17365214 -0.42434486 -2.16354639
n 0.59315079 -1.90803447 0.00000000
n -4.58176680 0.13383618 0.00000000
c 1.70910128 -2.35007145 0.00000000
c -5.69661674 0.57772701 0.00000000
c 3.29036523 0.37909604 0.00000000
c 0.69904423 1.39141245 0.00000000
c 2.64840286 0.63325866 -1.22864594
c 2.64840286 0.63325866 1.22864594
c 1.34253555 1.14290237 1.22908024
c 1.34253555 1.14290237 -1.22908024
h 3.17365214 0.42434486 -2.16354639
h 3.17365214 0.42434486 2.16354639
h 0.81899680 1.35630199 2.16447236
h 0.81899680 1.35630199 -2.16447236
n 4.58176680 -0.13383618 0.00000000
n -0.59315079 1.90803447 0.00000000
c 5.69661674 -0.57772701 0.00000000
c -1.70910128 2.35007145 0.00000000

aug-cc-pVTZ:
c -0.75174709 -1.39799615 0.00000000
c -3.30493425 -0.35414592 0.00000000
c -1.38576973 -1.13908529 -1.21702294
c -1.38576973 -1.13908529 1.21702294
c -2.67099928 -0.61427381 1.21653901
c -2.67099928 -0.61427381 -1.21653901
h -0.87034243 -1.35504522 -2.14306852
h -0.87034243 -1.35504522 2.14306852
h -3.18622049 -0.39850028 2.14215309
h -3.18622049 -0.39850028 -2.14215309
n 0.52622571 -1.92187353 0.00000000
n -4.57888461 0.17285859 0.00000000
c 1.62350129 -2.37186810 0.00000000
c -5.67638205 0.62048074 0.00000000
c 3.30493425 0.35414592 0.00000000
c 0.75174709 1.39799615 0.00000000
c 2.67099928 0.61427381 -1.21653901
c 2.67099928 0.61427381 1.21653901
c 1.38576973 1.13908529 1.21702294
c 1.38576973 1.13908529 -1.21702294
h 3.18622049 0.39850028 -2.14215309
h 3.18622049 0.39850028 2.14215309
h 0.87034243 1.35504522 2.14306852
h 0.87034243 1.35504522 -2.14306852
n 4.57888461 -0.17285859 0.00000000
n -0.52622571 1.92187353 0.00000000
c 5.67638205 -0.62048074 0.00000000
c -1.62350129 2.37186810 0.00000000

Parallel Displaced (**PD-57**)

aug-cc-pVDZ:
```
c 0.21707703 -1.76307300 -0.20605678
c -2.42911267 -0.89499935 -0.13207447
c -0.32815182 -1.11395553 -1.33114269
c -0.55184765 -1.98459322 0.95545007
c -1.88205525 -1.54543129 0.99401923
c -1.66069242 -0.67625563 -1.29314564
h 0.28849649 -0.96958774 -2.22142978
h -0.10356127 -2.50160602 1.80773239
h -2.50566657 -1.71050452 1.87603236
h -2.11595516 -0.17604976 -2.15182119
n 1.53127674 -2.21721111 -0.24811313
n -3.75827223 -0.49238205 -0.10641641
c 2.65328640 -2.64536489 -0.28164798
c -4.91067424 -0.15560298 -0.08642073
c 2.42911267 0.89499935 0.13207447
c -0.21707703 1.76307300 0.20605678
c 1.88205525 1.54543129 -0.99401923
c 1.66069242 0.67625563 1.29314564
c 0.32815182 1.11395553 1.33114269
c 0.55184765 1.98459322 -0.95545007
h 2.50566657 1.71050452 -1.87603236
h 2.11595516 0.17604976 2.15182119
h -0.28849649 0.96958774 2.22142978
h 0.10356127 2.50160602 -1.80773239
n 3.75827223 0.49238205 0.10641641
n -1.53127674 2.21721111 0.24811313
c 4.91067424 0.15560298 0.08642073
c -2.65328640 2.64536489 0.28164798
```

aug-cc-pVTZ:
```
C 0.13481600 -1.79045400 -0.19590700
C -2.46595200 -0.86322100 -0.12328500
C -0.39665500 -1.15131700 -1.31746000
C -0.62560900 -1.96804900 0.96293900
C -1.93187100 -1.50034600 1.00022500
C -1.70517600 -0.68539600 -1.28075300
H 0.21269900 -1.03461900 -2.20323900
H -0.18916700 -2.47247000 1.81442700
H -2.54629500 -1.62991700 1.88065500
H -2.14676400 -0.19130100 -2.13565200
N 1.43160200 -2.26217500 -0.23173200
N -3.77179100 -0.42360800 -0.09417700
C 2.53507500 -2.69799400 -0.25697600
C -4.90137700 -0.06301100 -0.07056300
C 2.46595200 0.86322100 0.12328500
C -0.13481600 1.79045400 0.19590700
C 1.93187100 1.50034600 -1.00022500
C 1.70517600 0.68539600 1.28075300
C 0.39665500 1.15131700 1.31746000
C 0.62560900 1.96804900 -0.96293900
H 2.54629500 1.62991700 -1.88065500
H 2.14676400 0.19130100 2.13565200
H -0.21269900 1.03461900 2.20323900
H 0.18916700 2.47247000 -1.81442700
N 3.77179100 0.42360800 0.09417700
N -1.43160200 2.26217500 0.23173200
C 4.90137700 0.06301100 0.07056300
C -2.53507500 2.69799400 0.25697600
```

T-Shaped I (**TI-0**)

aug-cc-pVDZ:
```
c 0.00000000 0.00000000 -2.10592204
c 0.00000000 0.00000000 -4.88670212
c 0.00000000 -1.22899905 -2.79524256
c 0.00000000 1.22899905 -2.79524256
c 0.00000000 1.22890584 -4.19682884
c 0.00000000 -1.22890584 -4.19682884
h 0.00000000 -2.16506879 -2.23181170
h 0.00000000 2.16506879 -2.23181170
h 0.00000000 2.16476755 -4.76044585
h 0.00000000 -2.16476755 -4.76044585
n 0.00000000 0.00000000 -0.71304647
n 0.00000000 0.00000000 -6.27889803
c 0.00000000 0.00000000 0.48631181
c 0.00000000 0.00000000 -7.47892362
c 1.38860682 0.00000000 3.50579328
c -1.38860682 0.00000000 3.50579328
c 0.70039524 -1.22814189 3.51485342
c 0.70039524 1.22814189 3.51485342
c -0.70039524 1.22814189 3.51485342
c -0.70039524 -1.22814189 3.51485342
h 1.26461834 -2.16371295 3.51289277
h 1.26461834 2.16371295 3.51289277
h -1.26461834 2.16371295 3.51289277
h -1.26461834 -2.16371295 3.51289277
n 2.78207774 0.00000000 3.48505340
n -2.78207774 0.00000000 3.48505340
c 3.98119220 0.00000000 3.45634090
c -3.98119220 0.00000000 3.45634090
```

aug-cc-pVTZ:
```
c 0.00000000 0.00000000 -2.13774367
c 0.00000000 0.00000000 -4.89404566
c 0.00000000 -1.21701239 -2.82141768
c 0.00000000 1.21701239 -2.82141768
c 0.00000000 1.21686603 -4.20947303
c 0.00000000 -1.21686603 -4.20947303
h 0.00000000 -2.14318409 -2.26398068
h 0.00000000 2.14318409 -2.26398068
h 0.00000000 2.14284423 -4.76714648
h 0.00000000 -2.14284423 -4.76714648
n 0.00000000 0.00000000 -0.75550899
n 0.00000000 0.00000000 -6.27518364
c 0.00000000 0.00000000 0.42901526
c 0.00000000 0.00000000 -7.46031714
c 1.37648686 0.00000000 3.52558982
c -1.37648686 0.00000000 3.52558982
c 0.69359411 -1.21618216 3.53246560
c 0.69359411 1.21618216 3.53246560
c -0.69359411 1.21618216 3.53246560
c -0.69359411 -1.21618216 3.53246560
h 1.25189641 -2.14194277 3.52984910
h 1.25189641 2.14194277 3.52984910
h -1.25189641 2.14194277 3.52984910
h -1.25189641 -2.14194277 3.52984910
n 2.75874942 0.00000000 3.50468728
n -2.75874942 0.00000000 3.50468728
c 3.94316190 0.00000000 3.47951403
c -3.94316190 0.00000000 3.47951403
```

T-Shaped I (**TI-90**)

aug-cc-pVDZ:
c 0.00000000 0.00000000 2.09861005
c 0.00000000 0.00000000 4.87857714
c 1.22948755 0.00000000 2.78727550
c -1.22948755 0.00000000 2.78727550
c -1.22906255 0.00000000 4.18892223
c 1.22906255 0.00000000 4.18892223
h 2.16536172 0.00000000 2.22338387
h -2.16536172 0.00000000 2.22338387
h -2.16487973 0.00000000 4.75264538
h 2.16487973 0.00000000 4.75264538
n 0.00000000 0.00000000 0.70567178
n 0.00000000 0.00000000 6.27087250
c 0.00000000 0.00000000 -0.49364854
c 0.00000000 0.00000000 7.47089239
c 1.38828152 0.00000000 -3.50279863
c -1.38828152 0.00000000 -3.50279863
c 0.70038488 1.22826820 -3.51298427
c 0.70038488 -1.22826820 -3.51298427
c -0.70038488 -1.22826820 -3.51298427
c -0.70038488 1.22826820 -3.51298427
h 1.26450108 2.16388233 -3.50971761
h 1.26450108 -2.16388233 -3.50971761
h -1.26450108 -2.16388233 -3.50971761
h -1.26450108 2.16388233 -3.50971761
n 2.78180365 0.00000000 -3.47473197
n -2.78180365 0.00000000 -3.47473197
c 3.98052276 0.00000000 -3.43355521
c -3.98052276 0.00000000 -3.43355521

aug-cc-pVTZ:
c 0.00000000 0.00000000 2.12965058
c 0.00000000 0.00000000 4.88535126
c 1.21741135 0.00000000 2.81278641
c -1.21741135 0.00000000 2.81278641
c -1.21699871 0.00000000 4.20089725
c 1.21699871 0.00000000 4.20089725
h 2.14355055 0.00000000 2.25507340
h -2.14355055 0.00000000 2.25507340
h -2.14302914 0.00000000 4.75851959
h 2.14302914 0.00000000 4.75851959
n 0.00000000 0.00000000 0.74737035
n 0.00000000 0.00000000 6.26655231
c 0.00000000 0.00000000 -0.43706737
c 0.00000000 0.00000000 7.45166371
c 1.37621606 0.00000000 -3.52135772
c -1.37621606 0.00000000 -3.52135772
c 0.69357582 1.21629550 -3.52946981
c 0.69357582 -1.21629550 -3.52946981
c -0.69357582 -1.21629550 -3.52946981
c -0.69357582 1.21629550 -3.52946981
h 1.25177600 2.14210512 -3.52564282
h 1.25177600 -2.14210512 -3.52564282
h -1.25177600 -2.14210512 -3.52564282
h -1.25177600 2.14210512 -3.52564282
n 2.75848666 0.00000000 -3.49366618
n -2.75848666 0.00000000 -3.49366618
c 3.94257119 0.00000000 -3.45699223
c -3.94257119 0.00000000 -3.45699223

T-Shaped II (**TII-0**)

aug-cc-pVDZ:
c 0.00000000 1.39227374 -2.36595073
c 0.00000000 -1.39227374 -2.36595073
c -1.22931342 0.70144352 -2.37950226
c 1.22931342 0.70144352 -2.37950226
c 1.22931342 -0.70144352 -2.37950226
c -1.22931342 -0.70144352 -2.37950226
h -2.16581443 1.26493448 -2.38690420
h 2.16581443 1.26493448 -2.38690420
h 2.16581443 -1.26493448 -2.38690420
h -2.16581443 -1.26493448 -2.38690420
n 0.00000000 2.78366023 -2.35130224
n 0.00000000 -2.78366023 -2.35130224
c 0.00000000 3.98385950 -2.33278834
c 0.00000000 -3.98385950 -2.33278834
c 1.39142078 0.00000000 2.36982302
c -1.39142078 0.00000000 2.36982302
c 0.70120613 0.00000000 3.59849037
c 0.70070249 0.00000000 1.14250759
c -0.70070249 0.00000000 1.14250759
c -0.70120613 0.00000000 3.59849037
h 1.26363765 0.00000000 4.53510033
h 1.25540125 0.00000000 0.20275739
h -1.25540125 0.00000000 0.20275739
h -1.26363765 0.00000000 4.53510033
n 2.78402265 0.00000000 2.36254546
n -2.78402265 0.00000000 2.36254546
c 3.98376340 0.00000000 2.33959703
c -3.98376340 0.00000000 2.33959703

aug-cc-pVTZ:
c 0.00000000 1.38027853 -2.38384227
c 0.00000000 -1.38027853 -2.38384227
c -1.21715171 0.69454652 -2.39326548
c 1.21715171 0.69454652 -2.39326548
c 1.21715171 -0.69454652 -2.39326548
c -1.21715171 -0.69454652 -2.39326548
h -2.14405543 1.25180825 -2.39792256
h 2.14405543 1.25180825 -2.39792256
h 2.14405543 -1.25180825 -2.39792256
h -2.14405543 -1.25180825 -2.39792256
n 0.00000000 2.76051220 -2.36980683
n 0.00000000 -2.76051220 -2.36980683
c 0.00000000 3.94596016 -2.35565835
c 0.00000000 -3.94596016 -2.35565835
c 1.37912235 0.00000000 2.38655054
c -1.37912235 0.00000000 2.38655054
c 0.69437219 0.00000000 3.60326853
c 0.69397990 0.00000000 1.17053219
c -0.69397990 0.00000000 1.17053219
c -0.69437219 0.00000000 3.60326853
h 1.25121539 0.00000000 4.52988471
h 1.24706933 0.00000000 0.24220536
h -1.24706933 0.00000000 0.24220536
h -1.25121539 0.00000000 4.52988471
n 2.76061823 0.00000000 2.37996051
n -2.76061823 0.00000000 2.37996051
c 3.94559360 0.00000000 2.35959648
c -3.94559360 0.00000000 2.35959648

T-Shaped II (**TII-90**)

aug-cc-pVDZ:
```
c -1.39234078 0.00000000 2.36621114
c 1.39234078 0.00000000 2.36621114
c -0.70123552 1.22926383 2.36448886
c -0.70123552 -1.22926383 2.36448886
c 0.70123552 -1.22926383 2.36448886
c 0.70123552 1.22926383 2.36448886
h -1.26480061 2.16542565 2.36446294
h -1.26480061 -2.16542565 2.36446294
h 1.26480061 -2.16542565 2.36446294
h 1.26480061 2.16542565 2.36446294
n -2.78361987 0.00000000 2.35978446
n 2.78361987 0.00000000 2.35978446
c -3.98437240 0.00000000 2.34770166
c 3.98437240 0.00000000 2.34770166
c -1.39206603 0.00000000 -2.36075973
c 1.39206603 0.00000000 -2.36075973
c -0.70098143 0.00000000 -3.58940717
c -0.70098110 0.00000000 -1.13350137
c 0.70098110 0.00000000 -1.13350137
c 0.70098143 0.00000000 -3.58940717
h -1.26399856 0.00000000 -4.52579042
h -1.25905715 0.00000000 -0.19558006
h 1.25905715 0.00000000 -0.19558006
h 1.26399856 0.00000000 -4.52579042
n -2.78412052 0.00000000 -2.35920354
n 2.78412052 0.00000000 -2.35920354
c -3.98447155 0.00000000 -2.36282977
c 3.98447155 0.00000000 -2.36282977
```

aug-cc-pVTZ:
```
c -1.38009033 0.00000000 2.39061574
c 1.38009033 0.00000000 2.39061574
c -0.69438198 1.21713438 2.38791235
c -0.69438198 -1.21713438 2.38791235
c 0.69438198 -1.21713438 2.38791235
c 0.69438198 1.21713438 2.38791235
h -1.25184207 2.14372796 2.38713101
h -1.25184207 -2.14372796 2.38713101
h 1.25184207 -2.14372796 2.38713101
h 1.25184207 2.14372796 2.38713101
n -2.76045611 0.00000000 2.38452867
n 2.76045611 0.00000000 2.38452867
c -3.94651373 0.00000000 2.37945892
c 3.94651373 0.00000000 2.37945892
c -1.38011518 0.00000000 -2.38529611
c 1.38011518 0.00000000 -2.38529611
c -0.69415055 0.00000000 -3.60172212
c -0.69432858 0.00000000 -1.16933608
c 0.69432858 0.00000000 -1.16933608
c 0.69415055 0.00000000 -3.60172212
h -1.25125703 0.00000000 -4.52819143
h -1.24973812 0.00000000 -0.24211006
h 1.24973812 0.00000000 -0.24211006
h 1.25125703 0.00000000 -4.52819143
n -2.76103619 0.00000000 -2.38456018
n 2.76103619 0.00000000 -2.38456018
c -3.94654607 0.00000000 -2.39130794
c 3.94654607 0.00000000 -2.39130794
```

Slipped-Parallel (**SP-2hb**)

aug-cc-pVDZ:
```
c 2.75976340 -0.86889921 0.00000000
c 5.34370310 0.14502293 0.00000000
c 2.94532897 0.52815432 0.00000000
c 3.84792310 -1.76371330 0.00000000
c 5.15260247 -1.25131409 0.00000000
c 4.25204772 1.03625371 0.00000000
h 2.07300423 1.18765163 0.00000000
h 3.66538704 -2.84094756 0.00000000
h 6.01977766 -1.91585086 0.00000000
h 4.43428678 2.11355994 0.00000000
n 1.46129281 -1.37878986 0.00000000
n 6.64072981 0.65368945 0.00000000
c 0.33561717 -1.78709012 0.00000000
c 7.75779983 1.09136994 0.00000000
c -5.34370310 -0.14502293 0.00000000
c -2.75976340 0.86889921 0.00000000
c -5.15260247 1.25131409 0.00000000
c -4.25204772 -1.03625371 0.00000000
c -2.94532897 -0.52815432 0.00000000
c -3.84792310 1.76371330 0.00000000
h -6.01977766 1.91585086 0.00000000
h -4.43428678 -2.11355994 0.00000000
h -2.07300423 -1.18765163 0.00000000
h -3.66538704 2.84094756 0.00000000
n -6.64072981 -0.65368945 0.00000000
n -1.46129281 1.37878986 0.00000000
c -7.75779983 -1.09136994 0.00000000
c -0.33561717 1.78709012 0.00000000
```

aug-cc-pVTZ:
```
c 2.74397853 -0.84479838 0.00000000
c 5.31238659 0.14229386 0.00000000
c 2.93827789 0.53783357 0.00000000
c 3.81672186 -1.73788051 0.00000000
c 5.11231030 -1.23955865 0.00000000
c 4.23615227 1.03177651 0.00000000
h 2.08033436 1.19788406 0.00000000
h 3.62848437 -2.80244377 0.00000000
h 5.96578072 -1.90293935 0.00000000
h 4.42426548 2.09645105 0.00000000
n 1.45257814 -1.34318406 0.00000000
n 6.60251271 0.63790283 0.00000000
c 0.33953489 -1.74339692 0.00000000
c 7.70915024 1.06136412 0.00000000
c -5.31238659 -0.14229386 0.00000000
c -2.74397853 0.84479838 0.00000000
c -5.11231030 1.23955865 0.00000000
c -4.23615227 -1.03177651 0.00000000
c -2.93827789 -0.53783357 0.00000000
c -3.81672186 1.73788051 0.00000000
h -5.96578072 1.90293935 0.00000000
h -4.42426548 -2.09645105 0.00000000
h -2.08033436 -1.19788406 0.00000000
h -3.62848437 2.80244377 0.00000000
n -6.60251271 -0.63790283 0.00000000
n -1.45257814 1.34318406 0.00000000
c -7.70915024 -1.06136412 0.00000000
c -0.33953489 1.74339692 0.00000000
```

Rotated-Parallel (**RP-0**)

aug-cc-pVDZ:
```
c 0.00000000 1.38718515 1.61441845
c 0.00000000 -1.38718515 1.61441845
c 1.23088688 0.70079418 1.64039286
c -1.23088688 0.70079418 1.64039286
c -1.23088688 -0.70079418 1.64039286
c 1.23088688 -0.70079418 1.64039286
n 0.00000000 2.77493275 1.51287016
n 0.00000000 -2.77493275 1.51287016
c 0.00000000 3.96699532 1.37038521
c 0.00000000 -3.96699532 1.37038521
h 2.16786293 1.26392541 1.63292338
h -2.16786293 1.26392541 1.63292338
h -2.16786293 -1.26392541 1.63292338
h 2.16786293 -1.26392541 1.63292338
c 1.38718515 0.00000000 -1.61441845
c -1.38718515 0.00000000 -1.61441845
c 0.70079418 1.23088688 -1.64039286
c 0.70079418 -1.23088688 -1.64039286
c -0.70079418 -1.23088688 -1.64039286
c -0.70079418 1.23088688 -1.64039286
n 2.77493275 0.00000000 -1.51287016
n -2.77493275 0.00000000 -1.51287016
c 3.96699532 0.00000000 -1.37038521
c -3.96699532 0.00000000 -1.37038521
h 1.26392541 2.16786293 -1.63292338
h 1.26392541 -2.16786293 -1.63292338
h -1.26392541 -2.16786293 -1.63292338
h -1.26392541 2.16786293 -1.63292338
```

aug-cc-pVTZ:
```
c 0.00000000 1.37634957 1.64482145
c 0.00000000 -1.37634957 1.64482145
c 1.21851538 0.69411287 1.66559536
c -1.21851538 0.69411287 1.66559536
c -1.21851538 -0.69411287 1.66559536
c 1.21851538 -0.69411287 1.66559536
n 0.00000000 2.75391245 1.55188305
n 0.00000000 -2.75391245 1.55188305
c 0.00000000 3.93236808 1.42060502
c 0.00000000 -3.93236808 1.42060502
h 2.14654503 1.24992632 1.65484009
h -2.14654503 1.24992632 1.65484009
h -2.14654503 -1.24992632 1.65484009
h 2.14654503 -1.24992632 1.65484009
c 1.37634957 0.00000000 -1.64482145
c -1.37634957 0.00000000 -1.64482145
c 0.69411287 1.21851538 -1.66559536
c 0.69411287 -1.21851538 -1.66559536
c -0.69411287 -1.21851538 -1.66559536
c -0.69411287 1.21851538 -1.66559536
n 2.75391245 0.00000000 -1.55188305
n -2.75391245 0.00000000 -1.55188305
c 3.93236808 0.00000000 -1.42060502
c -3.93236808 0.00000000 -1.42060502
h 1.24992632 2.14654503 -1.65484009
h 1.24992632 -2.14654503 -1.65484009
h -1.24992632 -2.14654503 -1.65484009
h -1.24992632 2.14654503 -1.65484009
```

tilt-T-Shaped (***tilt*-T-0**)

aug-cc-pVDZ:
```
c 2.31860686 0.41005091 1.39166051
c 2.31860686 0.41005091 -1.39166051
c 2.13248695 1.62673629 0.70126992
c 2.51651206 -0.80266342 0.70170827
c 2.51651206 -0.80266342 -0.70170827
c 2.13248695 1.62673629 -0.70126992
n 2.30053981 0.41000160 2.78351794
n 2.30053981 0.41000160 -2.78351794
c 2.27626262 0.41298833 3.98331951
c 2.27626262 0.41298833 -3.98331951
h 1.98790550 2.55123203 1.26554686
h 2.65012889 -1.73261410 1.25924821
h 2.65012889 -1.73261410 -1.25924821
h 1.98790550 2.55123203 -1.26554686
c -3.25362799 0.61070132 0.00000000
c -1.38248665 -1.44505904 0.00000000
c -3.69723514 -0.72732818 0.00000000
c -1.88046756 0.92733331 0.00000000
c -0.93710350 -0.10858160 0.00000000
c -2.75432276 -1.76482950 0.00000000
n -4.19082313 1.64020435 0.00000000
n -0.43769465 -2.46956833 0.00000000
c -4.99573452 2.53025684 0.00000000
c 0.41291699 -3.31527016 0.00000000
h -4.76873228 -0.94058950 0.00000000
h -1.56650143 1.97411793 0.00000000
h 0.13121771 0.10661146 0.00000000
h -3.06768747 -2.81141428 0.00000000
```

aug-cc-pVTZ:
```
c 2.32595260 0.48658858 1.37981503
c 2.32595260 0.48658858 -1.37981503
c 2.11603110 1.68682259 0.69436490
c 2.54109142 -0.71077473 0.69483734
c 2.54109142 -0.71077473 -0.69483734
c 2.11603110 1.68682259 -0.69436490
n 2.30896507 0.48650079 2.76053160
n 2.30896507 0.48650079 -2.76053160
c 2.28896767 0.49089935 3.94572641
c 2.28896767 0.49089935 -3.94572641
h 1.95545376 2.59906193 1.25252005
h 2.68871688 -1.62919335 1.24604222
h 2.68871688 -1.62919335 -1.24604222
h 1.95545376 2.59906193 -1.25252005
c -3.28701796 0.49144783 0.00000000
c -1.35536906 -1.47475957 0.00000000
c -3.67433023 -0.85033557 0.00000000
c -1.93923471 0.85590210 0.00000000
c -0.96648402 -0.13395592 0.00000000
c -2.70202963 -1.84149934 0.00000000
n -4.25512683 1.47638790 0.00000000
n -0.38070742 -2.45535075 0.00000000
c -5.08502784 2.32252188 0.00000000
c 0.48480773 -3.26452173 0.00000000
h -4.72571545 -1.10160967 0.00000000
h -1.66793597 1.90274008 0.00000000
h 0.08359864 0.11897788 0.00000000
h -2.97277708 -2.88814575 0.00000000
```

tilt-T-Shaped (***tilt*-T-90**)

aug-cc-pVDZ:
```
c -1.14424432 -2.21380441  0.00000000
c -2.91277849 -0.06092683  0.00000000
c -1.58514195 -1.68257018 -1.22952300
c -1.58514195 -1.68257018  1.22952300
c -2.47470028 -0.59777037  1.22902500
c -2.47470028 -0.59777037 -1.22902500
n -0.24260471 -3.27506919  0.00000000
n -3.81237814  0.99771573  0.00000000
c  0.55188639 -4.17514886  0.00000000
c -4.60295519  1.90135384  0.00000000
h -1.22596819 -2.11636113 -2.16589100
h -1.22596819 -2.11636113  2.16589100
h -2.83302244 -0.16240870  2.16483700
h -2.83302244 -0.16240870 -2.16483700
c  3.13529466  0.29642128  0.00000000
c  0.92755355  1.98770689  0.00000000
c  3.33222130  1.69279256  0.00000000
c  1.84117211 -0.26206214  0.00000000
c  0.73148482  0.59380424  0.00000000
c  2.22045155  2.54737433  0.00000000
n  4.24392435 -0.54555096  0.00000000
n -0.18959494  2.81944482  0.00000000
c  5.20280344 -1.26721316  0.00000000
c -1.16409274  3.52084201  0.00000000
h  4.34888381  2.09285734  0.00000000
h  1.72025603 -1.34888258  0.00000000
h -0.28460585  0.20211039  0.00000000
h  2.34334566  3.63291993  0.00000000
```

aug-cc-pVTZ:
```
C -1.26262700 -2.17105600  0.00000000
C -2.93979900  0.02356100  0.00000000
C -1.67922100 -1.62693400 -1.21723500
C -1.67922100 -1.62693400  1.21723500
C -2.52141200 -0.52221900  1.21677500
C -2.52141200 -0.52221900 -1.21677500
N -0.39903800 -3.24944300  0.00000000
N -3.79539500  1.10392600  0.00000000
C  0.35645400 -4.16353400  0.00000000
C -4.55303000  2.01637300  0.00000000
H -1.33721800 -2.06678200 -2.14406100
H -1.33721800 -2.06678200  2.14406100
H -2.85979000 -0.07879700  2.14308900
H -2.85979000 -0.07879700 -2.14308900
C  3.19279900  0.23291700  0.00000000
C  1.01092100  1.91973100  0.00000000
C  3.39231600  1.61570900  0.00000000
C  1.90753300 -0.31374300  0.00000000
C  0.81186500  0.53898600  0.00000000
C  2.29501400  2.46679200  0.00000000
N  4.28917100 -0.60680200  0.00000000
N -0.09289700  2.75077100  0.00000000
C  5.23521200 -1.32086600  0.00000000
C -1.04917700  3.45210100  0.00000000
H  4.40004800  2.00720700  0.00000000
H  1.78211600 -1.38891800  0.00000000
H -0.19636500  0.15393100  0.00000000
H  2.42167300  3.54046300  0.00000000
```