Supplementary Information

Fulminic Acid: A Quasibent Spectacle

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1. Quartic Force Field

Table S1. AE-CCSD(T)/CBS quartic force field of linear HCNO[a]

ij	F_{ij}	*ij*	F_{ij}	*ij*	F_{ij}
11	6.4872	31	–0.1027	44 = 66	0.0418
21	–0.1450	32	0.8325	54 = 76	0.1533
22	18.5293	33	11.1299	55 = 77	0.6763
ijk	F_{ijk}	*ijk*	F_{ijk}	*ijk*	F_{ijk}
111	–36.824	331	0.053	541 = 761	0.008
211	0.345	332	–1.331	542 = 762	0.546
221	–0.136	333	–89.507	543 = 763	–0.232
222	–118.835	441 = 661	–0.166	551 = 771	–0.036
311	0.046	442 = 662	–1.129	552 = 772	–1.767
321	–0.016	443 = 663	0.375	553 = 773	–1.564
322	–2.851				
ijkl	F_{ijkl}	*ijkl*	F_{ijkl}	*ijkl*	F_{ijkl}
1111	187.86	4411 = 6611	–0.013	5521 = 7721	–0.236
2111	1.331	4421 = 6621	0.156	5522 = 7722	–0.414
2211	–4.052	4422 = 6622	–0.938	5531 = 7731	–0.008
2221	1.802	4431 = 6631	–0.100	5532 = 7732	3.112
2222	636.69	4432 = 6632	0.544	5533 = 7733	2.127
3111	2.217	4433 = 6633	–0.150	5544 = 7766	–0.212
3211	–1.602	4444 = 6666	0.729	5554 = 7776	0.142
3221	–0.525	5421 = 7621	1.025	5555 = 7777	4.165
3222	5.095	5422 = 7622	0.477	7644	–0.008
3311	–1.992	5431 = 7631	1.044	7654	–0.031
3321	–0.998	5432 = 7632	0.364	7655	0.047
3322	3.305	5433 = 7633	–0.038	7744	–0.151
3331	2.782	5444 = 7666	–0.023	7754	0.047
3332	13.278	5511 = 7711	–0.223	7755	1.388
3333	529.53				

Internal coordinates: $S_1 = r$(H–C), $S_2 = r$(C–N), $S_3 = r$(N–O),
$S_4 = \theta_x$(H–C–N), $S_5 = \theta_x$(C–N–O), $S_6 = \theta_y$(H–C–N), $S_7 = \theta_y$(C–N–O)

[a]Units consistent with energy in aJ, bond distances in Å, and bond angles in rad. The linear bending angles are defined to have displacements of the same sign upon *cis*-bending. Reference geometry: [r_e(H–C), r_e(C–N), r_e(N–O)] = (1.05922, 1.15801, 1.20184) Å.

2. Total energies (in E_h) for the FPA computation of D_e(HCN–O)

Table S2. Linear HCNO total energies at the AE-CCSDTQ(P)/CBS + MVD1 reference geometry[a]

	ΔE_e(HF)	δ[MP2]	δ[Ć]	δ[Ć(T)]	δ[ĆT]	δ[ĆT(Q)]	δ[ĆTQ]	δ[ĆTQ(P)]	δ[ĆTQP]	δ[ĆTQP(H)]
6-31G* (FC)	–167.62739725	–168.10742976	–168.10529085	–168.12656949	–168.12660078	–168.12956504	–168.12903906	–168.12900408	–168.12923665	–168.12922970
cc-pVDZ (FC)	–167.64392020	–168.13514861	–168.13355834	–168.15559560	–168.15556096	–168.15858027	–168.15800830	–168.15795394		
cc-pVTZ (FC)	–167.69439791	–168.29809341	–168.28829116	–168.32107277	–168.32042252	–168.32356804				
cc-pCVQZ (FC)	–167.70751115	–168.35606474	–168.33934997	–168.37524662						
cc-pCVQZ (AE)	–167.70751115	–168.52167369	–168.50902170	–168.54651287						
cc-pCV5Z (AE)	–167.71034057	–168.54453598	–168.52733350	–168.56576292						
cc-pCV6Z (AE)	–167.71066768	–168.55372640	–168.53386159	–168.57263222						

[a]Ć is shorthand for CCSD. (FC, AE) specifies whether a given row pertains to (frozen-core, all-electron) computations.

Table S3. HCN total energies at the AE-CCSDTQ(P)/CBS + MVD1 reference geometry[a]

	ΔE_e(HF)	δ[MP2]	δ[Ć]	δ[Ć(T)]	δ[ĆT]	δ[ĆT(Q)]	δ[ĆTQ]	δ[ĆTQ(P)]	δ[ĆTQP]	δ[ĆTQP(H)]
6-31G* (FC)	–92.87336566	–93.15315906	–93.16185865	–93.17334771	–93.17356380	–93.17497209	–93.17477681	–93.17493646	–93.17492852	–93.17494007
cc-pVDZ (FC)	–92.88326275	–93.16737990	–93.17641216	–93.18826287	–93.18846522	–93.18989283	–93.18969166	–93.18985770		
cc-pVTZ (FC)	–92.90807939	–93.25321219	–93.25725008	–93.27511096	–93.27495945	–93.27653841				
cc-pCVQZ (FC)	–92.91459079	–93.28361553	–93.28329546	–93.30281495						
cc-pCVQZ (AE)	–92.91459079	–93.39079925	–93.39352052	–93.41408010						
cc-pCV5Z (AE)	–92.91574891	–93.40315363	–93.40308699	–93.42414416						
cc-pCV6Z (AE)	–92.91588156	–93.40826143	–93.40656597	–93.42780307						

[a]See footnote of Table S2.

Table S4. O(^3P) total energies[a]

	ΔE_e(HF)	δ[MP2]	δ[C]	δ[C(T)]	δ[CT]	δ[CT(Q)]	δ[CTQ]	δ[CTQ(P)]	δ[CTQP]	δ[CTQP(H)]
6-31G* (FC)	–74.78318092	–74.87815958	–74.89390972	–74.89474933	–74.89489554	–74.894942279	–74.89495186	–74.894954432	–74.89495492	–74.89495487
cc-pVDZ (FC)	–74.79216606	–74.89413156	–74.90920062	–74.90995028	–74.91006245	–74.91013058	–74.91014048	–74.91014266		
cc-pVTZ (FC)	–74.81175662	–74.95490238	–74.97105037	–74.97396183	–74.97425182	–74.974302711				
cc-pCVQZ (FC)	–74.81735974	–74.97674336	–74.99138896	–74.99516165						
cc-pCVQZ (AE)	–74.81735974	–75.03426423	–75.05001159	–75.05409082						
cc-pCV5Z (AE)	–74.81878776	–75.04261420	–75.05706347	–75.06140276						
cc-pCV6Z (AE)	–74.81894796	–74.81894796	–75.05945183	–75.06387986						

[a]See footnote of Table S2. UHF orbitals were employed for O(^3P), given that the spin contamination of the UHF reference wavefunction is negligible.