Supplemental Information for:

E/*Z* Energetics for Molecular Modeling and Design

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S1. G3 results for the RCOX set. Absolute energies are in Hartrees; relative energies are in kcal/mol; dipole moments are in Debye.

RCOX					
			G3		
Conformer	Name	E (0K)	H (298K)	G (298K)	μ
1a	(E)-acetic acid	-228.931838	-228.926252	-228.958740	4.9709
1b	(Z)-acetic acid	-228.939935	-228.934396	-228.966953	2.0394
	Δ (*E–Z)*	5.0809	5.1104	5.1537	2.9315
2a	(E)-*N*-methylacetamide	-248.324810	-248.317313	-248.354878	4.5357
2b	(Z)-*N*-methylacetamide	-248.328663	-248.320855	-248.359842	4.2161
	Δ (*E–Z)*	2.4178	2.2226	3.1150	0.3196
3a	(E)-methyl acetate	-268.184452	-268.177372	-268.213970	5.1725
3b	(Z)-methyl acetate	-268.196380	-268.189254	-268.225878	2.0763
	Δ (*E–Z)*	7.4849	7.4561	7.4724	3.0962
4a	(E)-methyl thioacetate	-591.051021	-591.043348	-591.081698	4.8330
4b	(Z)-methyl thioacetate	-591.058396	-591.050414	-591.091441	1.6890
	Normal mode correction (ΔS)[a]			-1.5138	
	Δ (*E–Z)*	4.6279	4.4340	4.6000	3.1440

[a] Using the freq = hindrot keyword with Gaussian 03. The correction was negligible for other structures.

S2. G3B3 results for the RCOX set. Absolute energies are in Hartrees; relative energies are in kcal/mol; dipole moments are in Debye.

RCOX					
			G3B3		
Conformer	Name	E (0K)	H (298K)	G(298K)	μ
1a	(E)-acetic acid	-228.936589	-228.930992	-228.963546	4.9215
1b	(Z)-acetic acid	-228.944725	-228.939142	-228.971939	2.0048
	Δ (*E–Z)*	5.1054	5.1142	5.2667	2.9167
2a	(E)-*N*-methylacetamide	-248.329932	-248.322416	-248.360068	4.4763
2b	(Z)-*N*-methylacetamide	-248.333663	-248.326011	-248.364323	4.1523
	Δ (*E–Z)*	2.3412	2.2559	2.6701	0.3240
3a	(E)-methyl acetate	-268.190111	-268.182912	-268.219971	5.1738
3b	(Z)-methyl acetate	-268.201940	-268.194717	-268.231797	2.0738
	Δ (*E–Z)*	7.4228	7.4078	7.4209	3.1000
4a	(E)-methyl thioacetate	-591.055948	-591.048174	-591.086699	4.7500
4b	(Z)-methyl thioacetate	-591.063320	-591.055208	-591.096092	1.5554
	Normal mode correction (ΔS)[a]			-1.5138	
	Δ (*E–Z)*	4.6260	4.4139	4.3804	3.1946

[a] Using the freq = hindrot keyword with Gaussian 03. The correction was negligible for other structures.

S3. G3B3 results for the RXCOYR set. Absolute energies are in Hartrees; relative energies are in kcal/mol; dipole moments are in Debye.

RXCOYR					
		G3B3			
Conformer	Name	E (0K)	H (298K)	G(298K	μ
5a	(E,Z)-1,3-dimethylurea	-303.653918	-303.645230	-303.685740	4.3865
5b	(Z,Z)-1,3-dimethylurea	-303.655604	-303.646871	-303.687471	3.8872
	Δ (*E–Z)*	1.0580	1.0297	1.0862	0.4993
6a	(E,Z)-1,3-dimethylthiourea	-626.502965	-626.493760	-626.536024	6.0248
6b	(Z,Z)-1,3-dimethylthiourea	-626.502696	-626.493610	-626.535140	5.2256
	Δ (*E–Z)*	-0.1688	-0.0941	-0.5547	0.7992
7a	(Z,E)-methyl *N*-methylcarbamate	-323.514800	-323.506452	-323.546275	5.5563
7b	(Z,Z)-methyl *N*-methylcarbamate	-323.526711	-323.518088	-323.559316	2.5102
	Δ (*E–Z)*	7.4743	7.3017	8.1834	3.0461
8a	(E,Z)-methyl *N*-methylcarbamate	-323.524732	-323.516259	-323.556523	2.8532
8b	(Z,Z)-methyl *N*-methylcarbamate	-323.526711	-323.518088	-323.559316	2.5102
	Δ (*E–Z)*	1.2418	1.1477	1.7526	0.3430
9a	(Z,E)-dimethylcarbonate	-343.384774	-343.376814	-343.415710	3.9735
9b	(Z,Z)-dimethylcarbonate	-343.389595	-343.381571	-343.420638	0.3722
	Δ (*E–Z)*	3.0252	2.9851	3.0924	3.6013

S4. G3B3 results for the C=C&N set. Absolute energies are in Hartrees; relative energies are in kcal/mol; dipole moments are in Debye.

C=C&N					
		G3B3			
Conformer	Name	E (0K)	H (298K)	G(298K	μ
10a	(E)-*N*-methyl-1-propen-2-amine	-212.370739	-212.363239	-212.400080	1.3968
10b	(Z)-*N*-methyl-1-propen-2-amine	-212.374990	-212.367465	-212.404229	1.5223
	Δ (*E–Z)*	2.6675	2.6519	2.6035	-0.1255
11a	(E)-2-methoxy-1-propene	-232.232764	-232.225401	-232.262204	2.0171
11b	(Z)-2-methoxy-1-propene	-232.239885	-232.232750	-232.268590	0.7430
	Δ (*E–Z)*	4.4685	4.6116	4.0073	1.2741
12a	cis-(E)-*N*,*N*'-dimethylacetimidamide	-267.699125	-267.690146	-267.730679	3.3513
12b	cis-(Z)-*N*,*N*'-dimethylacetimidamide	-267.692648	-267.683687	-267.724386	3.0451
	Δ (*E–Z)*	-4.0644	-4.0531	-3.9489	0.3062
13a	trans-(E)-*N*,*N*'-dimethylacetimidamide	-267.695834	-267.686733	-267.728033	2.4928
13b	trans-(Z)-*N*,*N*'-dimethylacetimidamide	-267.700824	-267.691508	-267.733511	2.5329
	Δ (*E–Z)*	3.1313	2.9964	3.4375	-0.0401
14a	trans-(E)-1-ethylidene-2-methylhydrazine	-228.394201	-228.386696	-228.423560	1.9430
14b	trans-(Z)-1-ethylidene-2-methylhydrazine	-228.393951	-228.386650	-228.423000	1.9544
	Δ (*E–Z)*	-0.1569	-0.0289	-0.3514	-0.0114
15a	cis-(E)-1-ethylidene-2-methylhydrazine	-228.393665	-228.386214	-228.423168	2.2405
15b	cis-(Z)-1-ethylidene-2-methylhydrazine	-228.388413	-228.381095	-228.417941	1.8734
	Δ (*E–Z)*	-3.2957	-3.2122	-3.2800	0.3671
16a	(E)-1-methyl-2-(propan-2-ylidene)hydrazine	-267.673477	-267.664521	-267.705040	2.1509
16b	(Z)-1-methyl-2-(propan-2-ylidene)hydrazine	-267.669435	-267.660641	-267.700761	1.6153
	Δ (*E–Z)*	-2.5364	-2.4347	-2.6851	0.5356
17a	(E)-propanone oxime	-248.268305	-248.260823	-248.298122	1.3071
17b	(Z)-propanone oxime	-248.258680	-248.251256	-248.287997	4.2439
	Δ (*E–Z)*	-6.0398	-6.0034	-6.3535	-2.9368
18a	(E)-*O*-methyl propanone oxime	-287.524908	-287.516510	-287.556573	1.1673
18b	(Z)-*O*-methyl propanone oxime	-287.494511	-287.487278	-287.524057	3.8296
	Δ (*E–Z)*	-19.0744	-18.3434	-20.4041	-2.6623