

Structural and Relative Energy Assessments of DFT Functionals and MP2 Method to Describe the Gas Phase Methylation of Nitronates: $[R^1R^2CNO_2]^- + CH_3I$

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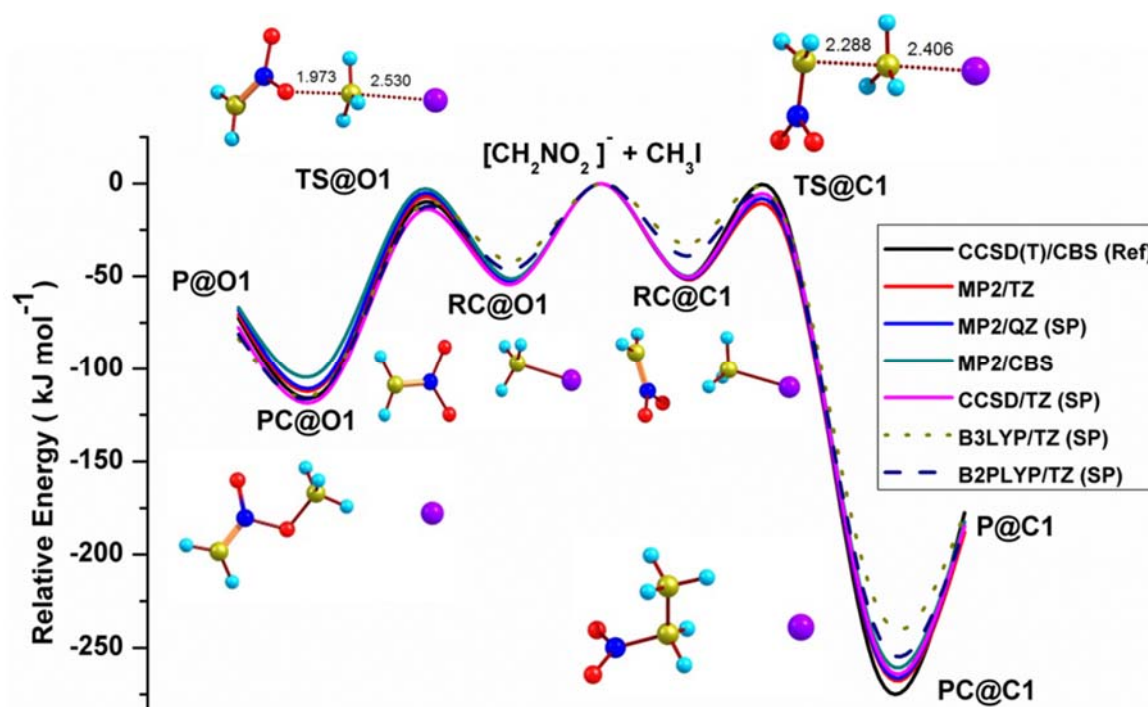


Figure S1. Energy profiles and selected structures (at the MP2/TZ level) of the $[\text{CH}_2\text{NO}_2]^-$ (**1**) + CH_3I reaction in the gas phase. The pathways through the oxygen (O-methylation or $\text{S}_{\text{N}}2@O$) and the carbon (C-methylation or $\text{S}_{\text{N}}2@C$) atoms of the nucleophile (nitronate) were considered. The calculations are single-point energies with selected methods and the reference CCSD(T)/CBS(D,T). Energies (in kJ mol^{-1}) include the zero-point vibrational corrections and distances are given in 10^{-10} m.

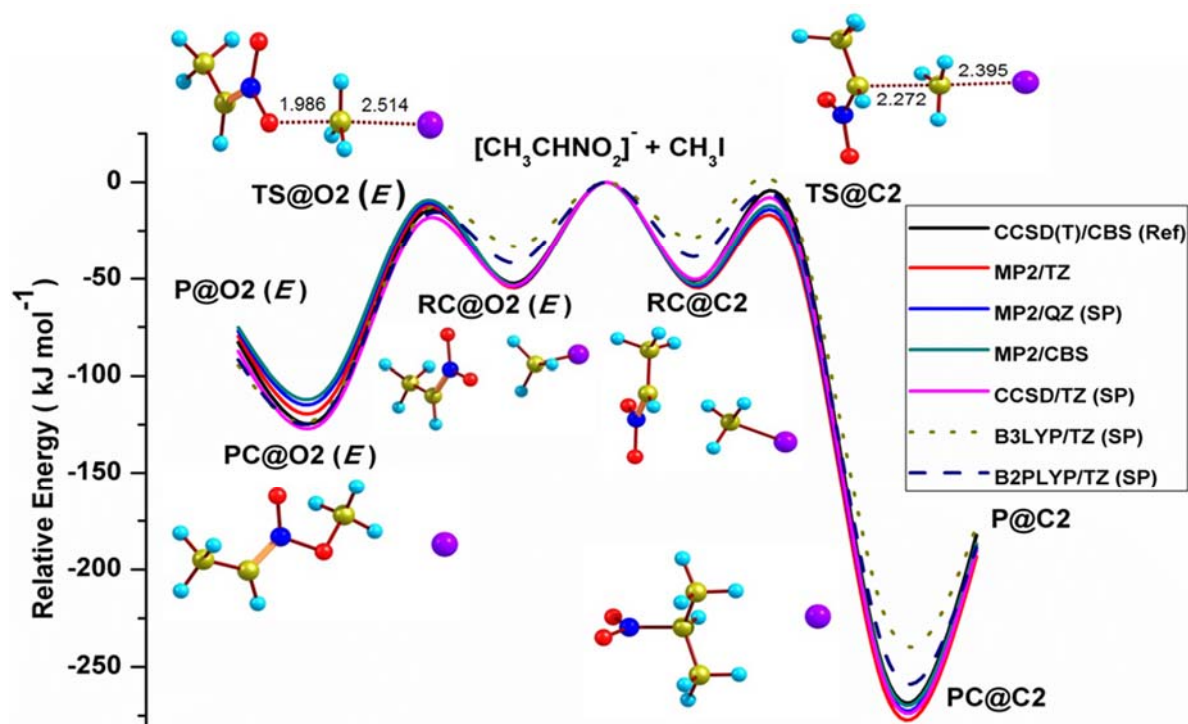


Figure S2. Same as Figure S1 for the $[\text{CH}_3\text{CHNO}_2]^-$ (2) + CH_3I reaction. The pathway yielding the *Z* stereoisomer, $\text{S}_{\text{N}}2@O2$ (*Z*), in the O-methylation pathway was omitted for clarity.

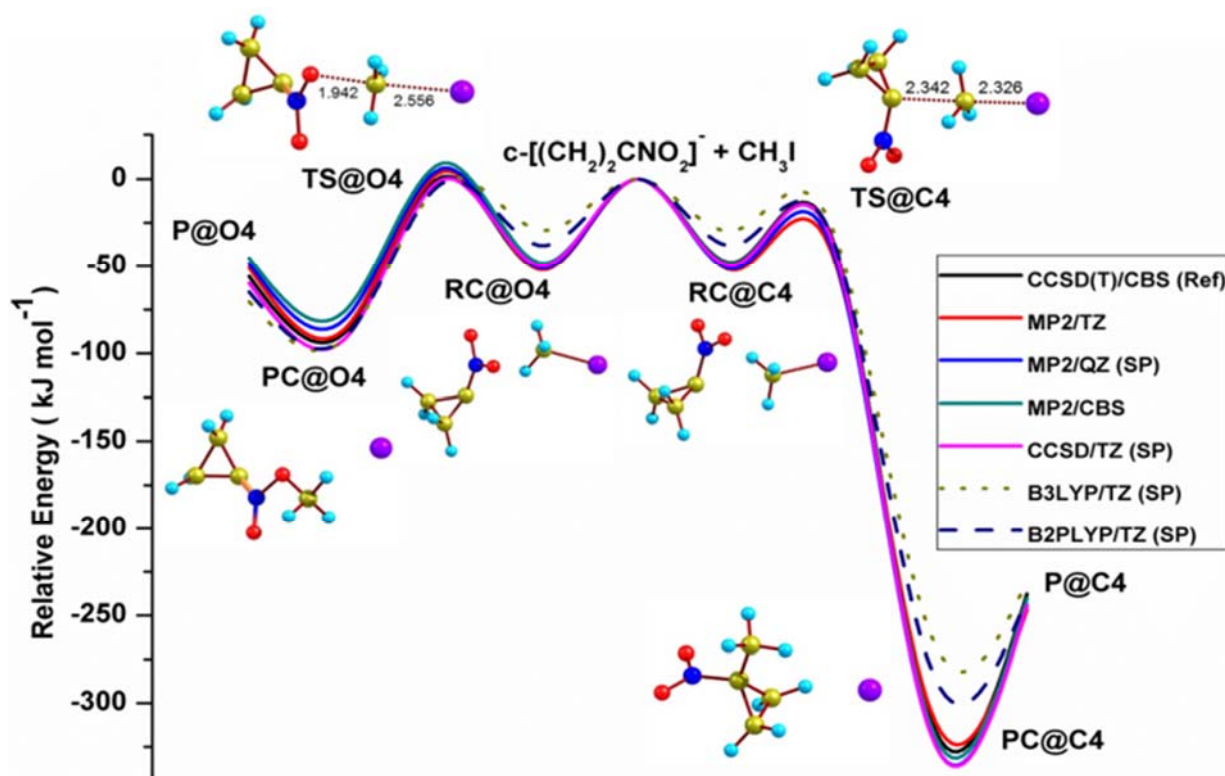


Figure S3. Same as Figure S1 for the $[c\text{-}(\text{CH}_2)_2\text{CNO}_2]^-$ (**4**) + CH_3I reaction.

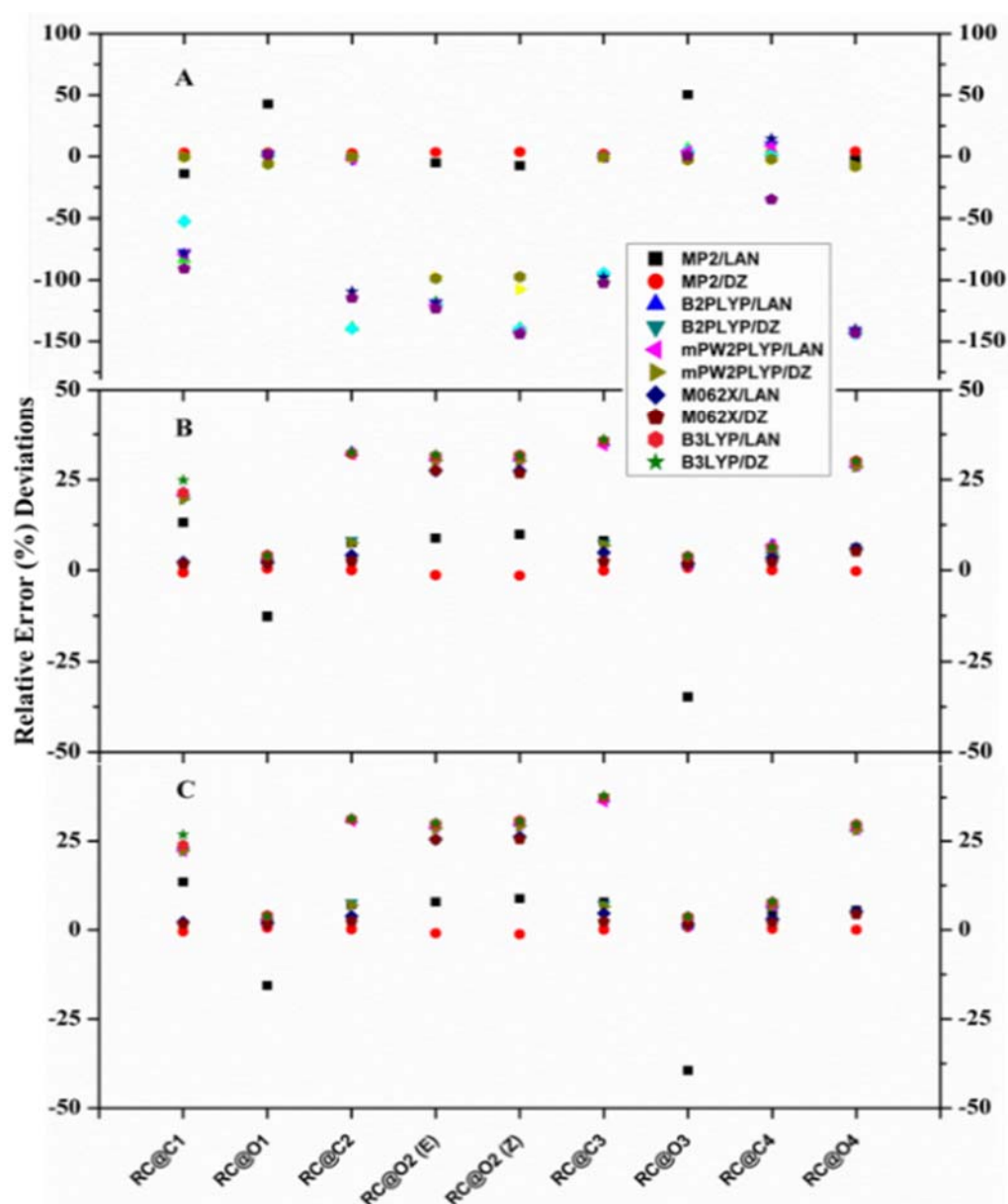


Figure S4. Relative error (%) deviations for the rotational constants of the reactant complexes (RCs) computed at the MP2/LAN (black squares), MP2/DZ (red circles), B2PLYP/LAN (blue triangles), B2PLYP/DZ (cadet blue triangles), mPW2PLYP/LAN (pink triangles), mPW2PLYP/DZ (olive triangles), M06-2X/LAN (dark blue squares), M06-2X/DZ (brown pentagons), B3LYP/LAN (red hexagons) and B3LYP/DZ (green stars) levels.

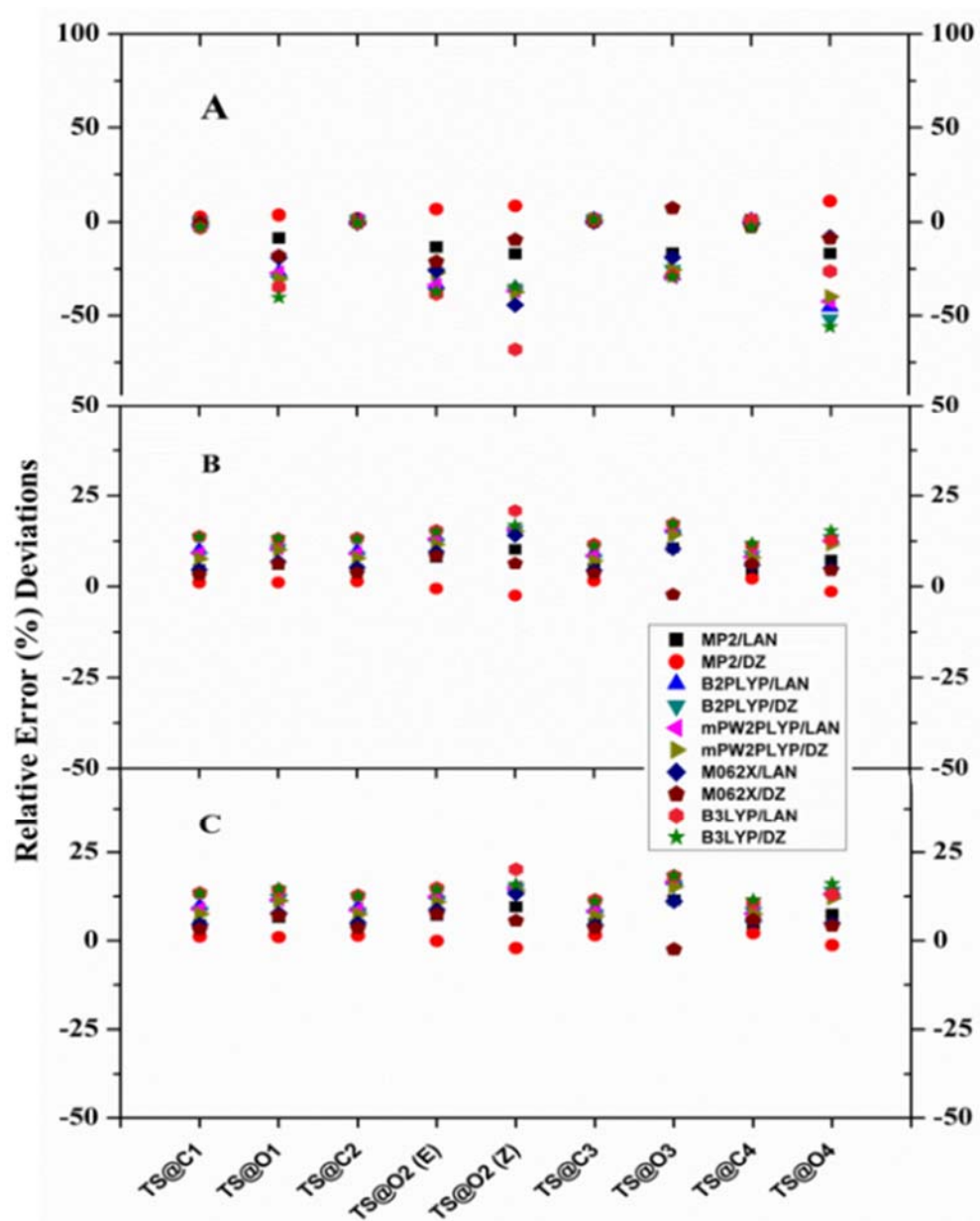


Figure S5. Relative error (%) deviations for the rotational constants of the reactant complexes (TSs) computed at the MP2/LAN (black squares), MP2/DZ (red circles), B2PLYP/LAN (blue triangles), B2PLYP/DZ (cadet blue triangles), mPW2PLYP/LAN (pink triangles), mPW2PLYP/DZ (olive triangles), M06-2X/LAN (dark blue squares), M06-2X/DZ (brown pentagons), B3LYP/LAN (red hexagons) and B3LYP/DZ (green stars) levels.

Table S1. The mean relative errors, MRE (%), in the rotational constants of RCs.

Rotational constant A										
RCs	MP2	MP2	B2PLY	B2PLYP	mPW2	mPW2	M062X/	M062X	B3LYP/	B3LYP
	/LAN	/DZ	P/LAN	/DZ	PLYP	PLYP	LAN	/DZ	LAN	/DZ
RC@C1	-0.14	0.03	-0.83	-0.78	-0.53	-0.79	-0.01	0.00	-0.79	-0.91
RC@O1	0.43	0.03	0.02	0.02	0.01	0.01	-0.06	-0.06	0.01	0.01
RC@C2	-0.01	0.02	-1.39	-0.02	-1.40	-0.02	-0.01	0.00	-1.09	-1.15
RC@O2 (E)	-0.05	0.03	-1.18	-1.19	-1.20	-1.20	-0.98	-0.99	-1.18	-1.23
RC@O2 (Z)	-0.07	0.04	-1.39	-1.41	-1.40	-1.43	-1.08	-0.98	-1.43	-1.44
RC@C3	-0.01	0.02	-0.99	0.00	-0.94	-0.01	-0.01	0.00	-0.98	-1.03
RC@O3	0.50	0.02	0.07	0.01	0.04	0.04	-0.03	-0.03	0.01	0.00
RC@C4	0.00	0.03	0.04	0.09	0.01	0.08	-0.03	-0.02	0.15	-0.35
RC@O4	-0.03	0.04	-1.42	-1.42	-1.44	-1.43	-0.08	-0.08	-1.40	-1.43
Rotational constant B										
RCs	MP2	MP2	B2PLY	B2PLYP	mPW2	mPW2	M062X/	M062X	B3LYP/	B3LYP
	/LAN	/DZ	P/LAN	/DZ	PLYP	PLYP	LAN	/DZ	LAN	/DZ
RC@C1	0.13	-0.01	0.21	0.20	0.21	0.20	0.02	0.02	0.21	0.25
RC@O1	-0.13	0.00	0.03	0.02	0.03	0.02	0.02	0.02	0.04	0.04
RC@C2	0.08	0.00	0.32	0.08	0.32	0.08	0.04	0.03	0.32	0.33
RC@O2 (E)	0.09	-0.01	0.31	0.31	0.31	0.30	0.27	0.28	0.32	0.32
RC@O2 (Z)	0.10	-0.02	0.31	0.31	0.31	0.30	0.27	0.27	0.32	0.32
RC@C3	0.08	0.00	0.35	0.07	0.34	0.07	0.05	0.02	0.36	0.36
RC@O3	-0.35	0.01	0.02	0.03	0.02	0.02	0.02	0.02	0.04	0.04
RC@C4	0.05	0.00	0.07	0.04	0.07	0.04	0.03	0.02	0.06	0.06
RC@O4	0.06	0.00	0.29	0.29	0.29	0.29	0.06	0.05	0.30	0.30
Rotational constant C										
RCs	MP2	MP2	B2PLY	B2PLYP	mPW2	mPW2	M062X/	M062X	B3LYP/	B3LYP
	/LAN	/DZ	P/LAN	/DZ	PLYP	PLYP	LAN	/DZ	LAN	/DZ
RC@C1	0.13	0.00	0.24	0.23	0.22	0.22	0.02	0.02	0.24	0.27
RC@O1	-0.16	0.01	0.03	0.02	0.03	0.02	0.02	0.02	0.04	0.04
RC@C2	0.07	0.00	0.31	0.08	0.31	0.07	0.04	0.02	0.31	0.31
RC@O2 (E)	0.08	-0.01	0.29	0.29	0.29	0.29	0.25	0.25	0.30	0.30
RC@O2 (Z)	0.09	-0.01	0.30	0.30	0.30	0.29	0.26	0.25	0.31	0.31
RC@C3	0.08	0.00	0.37	0.07	0.36	0.07	0.05	0.02	0.38	0.38
RC@O3	-0.39	0.01	0.01	0.03	0.01	0.01	0.02	0.02	0.04	0.04
RC@C4	0.05	0.00	0.07	0.07	0.07	0.07	0.03	0.02	0.08	0.08
RC@O4	0.05	0.00	0.29	0.28	0.28	0.28	0.05	0.04	0.30	0.30

Table S2. The mean relative errors, MRE (%), in the rotational constants of TSs.

Rotational constant A										
TSs	MP2		B2PL		mPW2P		mPW2		M062X	
	/LAN	/DZ	YP/L AN	B2PLYP /DZ	LYP /LAN	PLYP /DZ	M062X/ LAN	M062X /DZ	B3LYP/ LAN	B3LYP /DZ
TS@C1	0.01	0.02	-0.01	0.00	-0.01	0.00	-0.01	0.00	-0.03	-0.03
TS@O1	-0.09	0.04	-0.27	-0.31	-0.27	-0.30	-0.19	-0.18	-0.35	-0.40
TS@C2	0.01	0.02	0.00	0.01	0.00	0.00	-0.01	0.00	-0.01	-0.01
TS@O2 (E)	-0.13	0.07	-0.33	-0.27	-0.34	-0.27	-0.26	-0.21	-0.38	-0.37
TS@O2 (Z)	-0.17	0.08	-0.35	-0.37	-0.37	-0.37	-0.44	-0.10	-0.68	-0.34
TS@C3	0.01	0.02	0.01	0.01	0.01	0.01	0.00	0.00	0.01	0.01
TS@O3	-0.17	0.07	-0.28	-0.25	-0.29	-0.26	-0.19	0.07	-0.28	-0.29
TS@C4	0.01	0.01	0.01	0.00	0.00	-0.01	-0.01	-0.03	0.01	-0.03
TS@O4	-0.17	0.11	-0.45	-0.52	-0.42	-0.40	-0.08	-0.09	-0.26	-0.56
Rotational constant B										
TSs	MP2		B2PL		mPW2		mPW2		M062X	
	/LAN	/DZ	YP/L AN	B2PLYP /DZ	PLYP /LAN	PLYP /DZ	M062X/ LAN	M062X /DZ	B3LYP/L AN	B3LYP /DZ
TS@C1	0.05	0.01	0.10	0.08	0.09	0.08	0.05	0.03	0.14	0.14
TS@O1	0.06	0.01	0.11	0.11	0.11	0.10	0.07	0.06	0.13	0.13
TS@C2	0.05	0.01	0.10	0.09	0.09	0.08	0.05	0.04	0.13	0.13
TS@O2 (E)	0.08	-0.01	0.14	0.12	0.13	0.12	0.10	0.08	0.15	0.15
TS@O2 (Z)	0.10	-0.03	0.16	0.16	0.16	0.15	0.14	0.06	0.21	0.17
TS@C3	0.05	0.02	0.09	0.08	0.08	0.07	0.04	0.04	0.12	0.11
TS@O3	0.11	-0.02	0.16	0.15	0.15	0.14	0.10	-0.02	0.17	0.17
TS@C4	0.04	0.02	0.09	0.09	0.08	0.08	0.06	0.06	0.11	0.12
TS@O4	0.07	-0.01	0.13	0.13	0.13	0.12	0.05	0.04	0.13	0.15
Rotational constant C										
TSs	MP2		B2PL		mPW2		mPW2		M062X	
	/LAN	/DZ	YP/L AN	B2PLYP /DZ	PLYP /LAN	PLYP /DZ	M062X/ LAN	M062X /DZ	B3LYP/L AN	B3LYP /DZ
TS@C1	0.05	0.01	0.10	0.08	0.09	0.08	0.05	0.03	0.13	0.13
TS@O1	0.07	0.01	0.12	0.12	0.12	0.11	0.08	0.07	0.14	0.15
TS@C2	0.05	0.01	0.09	0.08	0.09	0.07	0.05	0.04	0.13	0.13
TS@O2 (E)	0.07	0.00	0.13	0.12	0.13	0.11	0.09	0.08	0.15	0.15
TS@O2 (Z)	0.10	-0.02	0.15	0.15	0.15	0.14	0.13	0.06	0.20	0.16
TS@C3	0.05	0.01	0.09	0.08	0.08	0.07	0.04	0.04	0.12	0.11
TS@O3	0.11	-0.02	0.17	0.16	0.17	0.15	0.11	-0.02	0.18	0.18
TS@C4	0.04	0.02	0.08	0.08	0.08	0.08	0.06	0.06	0.11	0.12
TS@O4	0.07	-0.01	0.14	0.14	0.13	0.12	0.05	0.04	0.13	0.16

Table S3. Relative energies (kcal mol⁻¹) for CCSD(T)/CBS results extrapolated from *aug-cc-pV{D,T}Z*-PP and *aug-cc-pV{T,Q}Z*-PP data for the [H₂CNO₂]⁻ + CH₃I reaction.

Stationary structure	CBS (D,T)	CBS (T,Q)	Difference
Available energy ($\Delta_{\text{RC}}E$) to RC@C	11.898	11.880	0.018
Available energy ($\Delta_{\text{RC}}E$) to RC@O	12.816	12.872	-0.056
Activation energy ($\Delta^\ddagger E$) @C	8.541	8.725	-0.184
Activation energy ($\Delta^\ddagger E$) @O	10.244	9.945	0.299
Energy of reaction ($\Delta_{\text{r}}E$) @C	-42.446	-43.191	0.744
Energy of reaction ($\Delta_{\text{r}}E$) @O	-17.379	-17.966	0.588

Cartesian coordinates (Å) of all stationary structures calculated at the MP2/aug-cc-pVTZ level, their energy (Eh in hartree) and lowest vibrational frequency (Frequency in cm⁻¹). Notation: RC = reactant complex, TS = transition state, PC = product complex.

CH₃I; Eh = -334.7447701; Frequency = 582.8419

C	-1.79410200	0.00000300	-0.00000800
H	-2.12494700	0.89171900	-0.51175100
H	-2.12489700	-0.88909400	-0.51633900
H	-2.12493900	-0.00266100	1.02812300
I	0.32338500	0.00000000	0.00000000

[CH₂NO₂]⁻; Eh = -244.1279287; Frequency = 373.0579

C	0.00006400	-1.29267900	0.00000000
H	0.00022800	-1.78191600	0.95287400
H	0.00022800	-1.78191600	-0.95287400
N	-0.00026700	0.04792300	0.00000000
O	0.00006400	0.68652800	-1.10183000
O	0.00006400	0.68652800	1.10183000

RC@C1; Eh = -578.7808029; Frequency = 42.7030

C	-0.21838400	0.56068100	-0.00000200
H	-0.22316000	1.64227500	-0.00001400
H	-0.68162400	0.14154400	-0.88678800
H	-0.68162200	0.14156400	0.88679300
I	1.83565600	-0.03263700	0.00000200
C	-3.38362200	1.13808500	-0.00001300

H	-3.57085400	1.59212700	-0.95637600
H	-3.57086100	1.59214200	0.95634200
N	-3.04158700	-0.16255600	-0.00000200
O	-2.85366100	-0.77715300	1.10624900
O	-2.85365400	-0.77717000	-1.10624200

RC@O1; Eh = -578.7810558; Frequency = 45.2039

C	0.03674700	-0.52372800	-0.00047900
H	0.19524600	-1.11234800	-0.89365700
H	0.65811900	0.36615400	-0.00080100
H	0.19586700	-1.11215900	0.89271400
I	-2.03166000	0.05876200	0.00018000
C	4.72677800	0.13614900	0.00180100
H	5.15909300	1.11982400	0.00228300
H	5.27056800	-0.79060200	0.00269200
N	3.38964000	0.05768500	-0.00021300
O	2.80679900	-1.08495700	-0.00095100
O	2.67950400	1.12700900	-0.00144800

TS@C1; Eh = -578.7710298; Frequency = -487.7052

C	-0.43561300	0.58636000	-0.00000600
H	-0.23176200	1.64067400	-0.00001500
H	-0.71705900	0.10829100	-0.92313800
H	-0.71706100	0.10830800	0.92313500

I	1.87698700	-0.07903700	0.00000200
C	-2.64058900	1.19627900	-0.00001300
H	-2.75020200	1.70962200	-0.94190100
H	-2.75020300	1.70964000	0.94186500
N	-3.10425200	-0.09467600	-0.00000100
O	-3.25794300	-0.69503100	1.10207500
O	-3.25794100	-0.69505100	-1.10206700

TS@O1; Eh = -578.764673; Frequency = -553.7387

C	0.53099500	-0.31452800	-0.42507000
H	0.28649000	-0.95179100	-1.25179500
H	0.69723500	0.73447800	-0.57998500
H	0.68613000	-0.74269500	0.54771800
I	-1.92440200	0.02793300	0.08138700
C	3.86300800	-0.50437600	0.90333300
H	4.44946700	0.13751400	1.53569700
H	3.84750700	-1.57739700	0.93460300
N	3.12533900	0.08741500	-0.03346400
O	2.42324100	-0.68482300	-0.84164000
O	3.04989400	1.33744100	-0.17524900

PC@C1; Eh = -578.8622099; Frequency = 24.4482

C	1.43781200	1.51082300	-0.00028600
H	0.36371300	1.69462500	-0.00030800
H	1.88661500	1.95026400	-0.89049700
H	1.88664500	1.95061900	0.88973400

I	-1.97451200	-0.09757900	0.00001900
C	1.61582400	0.00518000	0.00001100
H	1.18858200	-0.44668500	-0.88848100
H	1.18860600	-0.44633100	0.88869400
N	3.07365600	-0.30646100	0.00005600
O	3.64362100	-0.40482700	1.08945600
O	3.64357700	-0.40537000	-1.08931800

PC@O1; Eh = -578.8043176; Frequency = 27.3337

C	-1.41449800	0.68035600	0.00021300
H	-0.42097400	0.22971800	0.00022200
H	-1.55898800	1.28461400	0.89231100
H	-1.55868100	1.28523700	-0.89150500
I	2.34097600	-0.04937100	0.00004200
C	-4.47717100	-1.09086000	0.00029800
H	-5.52748600	-0.86801600	0.00027200
H	-4.02874300	-2.06553300	0.00059700
N	-3.66438800	-0.05397100	-0.00014900
O	-2.31041000	-0.44535200	-0.00031300
O	-3.93660700	1.14428500	-0.00045400

P@C1; Eh = -283.8721131; Frequency = 25.7666

C	-1.75941800	0.00003000	-0.42035900
H	-2.75831500	-0.00010900	0.01142200
H	-1.64889500	-0.88727600	-1.04039600
H	-1.64895900	0.88763300	-1.03998100

C	-0.72878800	-0.00019100	0.69315600
H	-0.78637100	-0.89625600	1.30355200
H	-0.78644400	0.89559100	1.30396200
N	0.63048900	0.00000600	0.08167700
O	1.13392500	1.09378300	-0.17160100
O	1.13417400	-1.09361600	-0.17178400

P@O1; Eh = -283.8250448; Frequency = 37.3331

C	1.77632600	-0.05790700	0.00029100
H	2.52669800	-0.84315600	-0.00013000
H	1.87193300	0.55841500	0.89099000
H	1.87232300	0.55974500	-0.88943500
C	-1.71111600	-0.54811600	0.00013300
H	-2.60258600	0.05097600	0.00026800
H	-1.66055600	-1.61969900	0.00006900
N	-0.57477200	0.10903900	-0.00004700
O	0.54906900	-0.78896100	-0.00051300
O	-0.34602800	1.30978400	0.00001600

[CH₃CHNO₂]⁻; Eh = -283.2922203; Frequency = 165.9370

C	0.56074500	-0.72129400	0.00007100
H	0.43264800	-1.79027800	-0.00004500
N	-0.57160000	0.00101000	0.00001600
O	-1.71915300	-0.57184700	-0.00002800
O	-0.48756400	1.28218600	0.00000500
C	1.86772400	-0.01617400	-0.00002400

H	2.68198500	-0.74513500	-0.00032500
H	1.98455400	0.63538900	-0.87369700
H	1.98492900	0.63505400	0.87384700

RC@C2; Eh = -618.0110363; Frequency = 39.5688

C	0.00353000	0.23246500	-0.33689500
H	0.11990500	1.10527800	-0.96564200
H	0.48934400	0.34332500	0.62658100
H	0.34037600	-0.67970800	-0.81875800
I	-2.09681800	0.03456000	0.02764900
C	3.01435000	0.43667100	-0.66839100
H	3.10429000	0.29222400	-1.73189000
N	2.69933800	-0.66010600	0.04051800
O	2.45185900	-1.77331100	-0.54653000
O	2.59736700	-0.56433100	1.31615800
C	3.27540100	1.71039600	0.04799300
H	3.53755800	2.49172200	-0.66870600
H	2.40221700	2.04528400	0.62094400
H	4.08882200	1.61488200	0.77516300

RC@O2 (Z); Eh = -618.0112681; Frequency = 27.3213

C	-0.09772500	-0.22688500	0.61178300
H	-0.15659200	-0.47427000	1.66265200
H	0.33055000	-1.03516100	0.02588600
H	0.44182500	0.69719900	0.44807900
I	-2.10453300	0.09549600	-0.06360100

C	3.03846100	0.48476500	-0.76465200
H	3.03091400	0.39052700	-1.83709700
N	2.69665500	-0.61836700	-0.08327200
O	2.68293200	-0.57803500	1.20047500
O	2.34050700	-1.69198000	-0.69279800
C	3.43059200	1.70311500	-0.01162100
H	3.68185300	2.50526500	-0.70853800
H	2.62785200	2.05440900	0.64715600
H	4.29176300	1.52346400	0.64113500

RC@O2 (E); Eh = -618.0110002; Frequency = 18.3058

C	0.18782100	-0.81984100	-0.16912100
H	0.38615400	-1.87219000	-0.31778400
H	-0.36684900	-0.63392400	0.74478500
H	-0.31588300	-0.38349800	-1.02200000
I	2.09068400	0.15249300	0.00152700
C	-3.11701400	0.46249100	-0.70302300
H	-3.29399700	0.21566800	-1.73624800
N	-2.71751500	-0.55588200	0.07272500
O	-2.48798600	-1.71746500	-0.42454900
O	-2.52083000	-0.34750700	1.32590000
C	-3.37201200	1.78776600	-0.08219800
H	-2.48076500	2.17976100	0.41783700
H	-3.68321300	2.50136900	-0.84789800
H	-4.15133500	1.73916400	0.68653300

TS@C2; Eh = -618.0329876; Frequency = -485.1534

C	0.24929400	0.24828500	-0.32781300
H	0.15062300	1.17597000	-0.86216400
H	0.55072300	0.27601100	0.70715500
H	0.41335200	-0.66448500	-0.87690400
I	-2.09732400	-0.03418600	0.04672500
C	2.46850900	0.55498600	-0.64963000
H	2.51292800	0.44739900	-1.72313900
N	2.81214800	-0.59291400	0.01509100
O	2.78123100	-1.70219900	-0.59652300
O	3.05247800	-0.52572300	1.25844400
C	2.74104500	1.85561800	0.02337200
H	2.45691600	2.67434900	-0.64088100
H	2.16983200	1.94778800	0.94987300
H	3.79598400	1.97527500	0.29307400

TS@O2 (Z) ; Eh = -618.0236675; Frequency = -559.3264

C	-0.22507100	0.10199400	0.53460300
H	0.00082800	-0.16990600	1.54668200
H	-0.27381400	1.13515000	0.24607400
H	-0.46865100	-0.66212500	-0.17936100
I	2.22153500	-0.08199100	-0.08906700
C	-3.54903900	-0.22839000	-0.62941700
H	-4.07565500	0.19273800	-1.46993800
N	-2.75882800	0.62727900	0.01672700

O	-2.11634100	0.16672900	1.07775800
O	-2.57612100	1.82748500	-0.33473300
C	-3.70075100	-1.62531800	-0.14418500
H	-4.36274600	-2.17397900	-0.81514900
H	-2.74190600	-2.14686100	-0.10069000
H	-4.11875600	-1.66389100	0.86562200

TS@O2 (E) ; Eh = -618.0256609; Frequency = -548.5502

C	0.08023300	0.68889900	-0.20630300
H	-0.27280200	1.60741000	-0.63211400
H	0.26416900	0.61973000	0.84917400
H	0.34529000	-0.12867800	-0.85064000
I	-2.26789100	-0.18052800	0.01236000
C	3.42092600	-0.29333600	-0.71463400
H	3.32006800	-0.10496200	-1.76912200
N	2.69929600	0.49226100	0.08181300
O	1.91096400	1.39950000	-0.46638000
O	2.72560300	0.37914900	1.34211100
C	4.31650000	-1.29869400	-0.09103300
H	3.75335300	-1.99656500	0.53480800
H	4.84397500	-1.86079200	-0.86145900
H	5.05061100	-0.82438200	0.56755800

PC@C2; Eh = -618.0948346; Frequency = 20.8733

C	1.33439200	0.83677200	1.26096500
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H	0.25922500	1.02067900	1.27405000
H	1.88484600	1.77694200	1.25456900
H	1.60174700	0.26564700	2.15050500
I	-2.14951900	-0.09618400	-0.00013000
C	1.62364000	0.04779700	-0.00001300
H	1.06847900	-0.88666400	-0.00131600
N	3.07217800	-0.35133800	-0.00046100
O	3.34783900	-1.55389600	-0.00166200
O	3.91511000	0.54831500	0.00046200
C	1.33450200	0.84024900	-1.25878900
H	0.25932300	1.02426800	-1.27134800
H	1.88498600	1.78042200	-1.24982600
H	1.60186800	0.27157600	-2.14989300

PC@O2 (Z) ; Eh = -618.0387569; Frequency = 26.1066

C	1.49584100	-1.75463000	0.52957300
H	1.31241100	-2.26563900	1.47050800
H	2.07313500	-2.38733300	-0.14226200
H	0.54837300	-1.43633000	0.08963800
I	-1.95619500	-0.04068000	-0.09523200
C	2.22993500	1.32353300	-0.32078900
H	2.57292900	1.84969300	-1.19851400
N	2.66315600	0.08371700	-0.28039500
O	2.27531000	-0.60047500	0.90422000
O	3.37647000	-0.53634800	-1.07905500
C	1.29915700	1.89275900	0.68752900

H	1.15802700	2.95105300	0.47434300
H	0.32110500	1.39838700	0.63686800
H	1.68642100	1.78479900	1.70027600

PC@O2 (E) ; Eh = -618.0358799; Frequency = 20.4186

C	-0.91326300	-0.74959600	0.09717800
H	0.06643800	-0.34790300	-0.16179700
H	-1.05344600	-1.74135800	-0.32246500
H	-1.02547700	-0.77486000	1.18065100
I	2.82063200	0.09319000	0.02362300
C	-3.96474000	0.89392400	-0.01232200
H	-3.48322100	1.84874600	-0.12375100
N	-3.17683600	-0.15554800	-0.12333300
O	-1.85502100	0.18118200	-0.47337700
O	-3.48449200	-1.34438500	0.00051000
C	-5.40622400	0.64690600	0.23552100
H	-5.56166400	0.14362700	1.19271500
H	-5.95201100	1.58735100	0.23945600
H	-5.82477800	-0.00761800	-0.53282400

P@C2; Eh = -323.1029393; Frequency = 27.2995

C	-1.26132400	-1.26403200	0.01710600
H	-2.27941200	-1.29490800	-0.36839600
H	-1.29529600	-1.26848300	1.10487000
H	-0.73399700	-2.15270500	-0.32660100
C	-0.58478900	0.00046800	-0.47670000

H	-0.48656700	0.00144900	-1.55959500
N	0.83454400	-0.00019300	0.01601400
O	1.73279200	0.00109200	-0.82619600
O	1.00486500	-0.00182700	1.23378100
C	-1.26076200	1.26440100	0.01937600
H	-2.27851800	1.29690100	-0.36685800
H	-1.29553900	1.26654400	1.10712200
H	-0.73248500	2.15340900	-0.32201300

P@O2 (Z) ; Eh = -323.0546246; Frequency = 62.1713

C	-1.95164200	-0.76958700	-0.00004600
H	-2.21006600	-1.82461200	-0.00010000
H	-2.34161700	-0.28124600	-0.88965500
H	-2.34180200	-0.28129600	0.88950700
C	1.31498300	0.55806200	0.00002700
H	1.72833300	1.55302000	-0.00002400
N	-0.00137500	0.55154800	0.00002000
O	-0.52211000	-0.79036500	0.00009700
O	-0.80604900	1.47728800	-0.00001500
C	2.10953600	-0.69796700	-0.00004000
H	3.16738400	-0.44700100	-0.00008900
H	1.89776600	-1.30909100	0.87804200
H	1.89762900	-1.30904500	-0.87811800

P@O2 (E) ; Eh = -323.0575299; Frequency = 37.6545

C	-2.28532600	0.02026700	0.18127600
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H	-3.11174000	-0.66557900	0.02014900
H	-2.39987500	0.90565900	-0.43757500
H	-2.22761100	0.30441200	1.23145100
C	1.13152600	-0.68900000	0.03192500
H	0.96815400	-1.75154400	0.05599900
N	0.04927400	0.04780800	-0.07205200
O	-1.14232100	-0.74421200	-0.20819200
O	-0.05716000	1.27051300	-0.09954900
C	2.43791100	0.01233600	0.08628600
H	2.50030100	0.65753800	0.96485500
H	3.24760000	-0.71114100	0.12182300
H	2.56942700	0.65397400	-0.78733300

$[(\text{CH}_3)_2\text{CNO}_2]^-$; Eh = -322.5219423; Frequency = 95.0510

C	-0.00061300	-0.58913600	0.00000000
N	-0.00012900	0.75394300	0.00000000
O	0.00010400	1.39046700	-1.11876500
O	0.00010400	1.39046700	1.11876500
C	0.00010400	-1.27363500	-1.32128300
H	0.87424600	-1.00014100	-1.92403000
H	-0.00273400	-2.35741400	-1.18219700
H	-0.87067400	-0.99576400	-1.92673800
C	0.00010400	-1.27363500	1.32128300
H	0.87424600	-1.00014100	1.92403000
H	-0.87067400	-0.99576400	1.92673800
H	-0.00273400	-2.35741400	1.18219700

RC@C3; Eh = -657.2424471; Frequency = 49.7520

C	0.17098600	-0.22808700	-0.00005200
H	-0.03500700	-1.29088200	-0.00087300
H	-0.19814400	0.27034700	0.89064900
H	-0.19845700	0.27186700	-0.88974500
I	2.30429000	-0.03491300	-0.00007100
C	-2.73741500	-0.49199500	-0.00020600
N	-2.45545400	0.82346500	0.00056300
O	-2.29713000	1.43934100	-1.11713400
O	-2.29584300	1.43778600	1.11893300
C	-2.89587200	-1.15618700	-1.32181800
H	-1.97970800	-1.09793000	-1.92300800
H	-3.15384100	-2.20833400	-1.18403600
H	-3.67314200	-0.67790600	-1.92719900
C	-2.89590100	-1.15808300	1.32040400
H	-1.98039300	-1.10074500	1.92269000
H	-3.67380900	-0.68110400	1.92607000
H	-3.15367800	-2.21007100	1.18093200

RC@O3; Eh = -657.2404725; Frequency = 4.3871

C	-0.77039200	-0.54573000	0.00030500
H	-0.62124900	-1.13664300	0.89355000
H	-0.13627100	0.33560800	0.00041300
H	-0.62095000	-1.13664600	-0.89288900
I	-2.83086700	0.06697000	-0.00004600

C	3.90924400	0.06422500	-0.00009700
N	2.57221900	-0.00176700	0.00020400
O	1.98395600	-1.15050000	0.00024200
O	1.87578800	1.08596000	0.00050600
C	4.52706800	1.41828300	-0.00022200
H	4.21996000	2.00505700	0.87228800
H	5.61558600	1.33312900	-0.00011000
H	4.22016400	2.00488200	-0.87293500
C	4.65575500	-1.22327700	-0.00053800
H	4.40713600	-1.83742500	0.87187800
H	4.40717300	-1.83686900	-0.87337000
H	5.73084400	-1.03283000	-0.00047500

TS@C3; Eh = -657.2658465; Frequency = -465.3138

C	0.07758100	0.24333300	0.00002600
H	0.05324200	1.31934600	0.00012500
H	0.28071900	-0.27523300	0.92401200
H	0.28079300	-0.27506100	-0.92404100
I	-2.28541400	-0.03699000	-0.00009500
C	2.30974400	0.56803700	0.00014600
N	2.57898000	-0.77994600	0.00003100
O	2.65524900	-1.39597500	-1.10810200
O	2.65516000	-1.39618200	1.10805400
C	2.51805600	1.27778200	-1.29642100
H	1.97133800	0.79004000	-2.10332400
H	2.17265200	2.31017600	-1.20659700

H	3.57425000	1.29430800	-1.59465500
C	2.51795200	1.27754000	1.29686100
H	1.97117000	0.78964800	2.10362900
H	3.57412200	1.29401000	1.59518300
H	2.17255500	2.30995100	1.20720200

TS@O3; Eh = -657.225167; Frequency = -545.7739

C	-0.15063900	0.00507300	-0.70102700
H	0.16670100	0.66551500	0.08402500
H	-0.05056600	-1.05669700	-0.57449500
H	-0.46883900	0.41127300	-1.64086700
I	-2.50962900	0.03476300	0.17873700
C	3.18748000	0.30678000	0.27944700
N	2.42858200	-0.49325100	-0.47118400
O	1.69899800	0.05768700	-1.42751400
O	2.36382600	-1.74716000	-0.28468200
C	4.01323700	-0.36080800	1.32237600
H	4.70072600	-1.08961100	0.88039600
H	4.58896800	0.37842300	1.87927500
H	3.38719500	-0.92600500	2.01847800
C	3.20763700	1.76466400	-0.03096500
H	3.59660900	1.96283700	-1.03453700
H	2.20645700	2.20042000	-0.00239100
H	3.83415400	2.28569200	0.69391800

PC@C3; Eh = -657.3273309; Frequency = 37.5198

C	-1.25082300	-0.69213400	-1.25301800
H	-0.15802100	-0.67237400	-1.24980900
H	-1.61790400	-0.18702800	-2.14833900
H	-1.60055800	-1.72308900	-1.25016700
I	2.39072000	-0.00496100	-0.00004800
C	-1.71628300	0.03488900	0.00023300
N	-3.23968000	-0.01299700	0.00008900
O	-3.76734200	-1.12694600	-0.00013600
O	-3.87567500	1.04377500	-0.00018100
C	-1.25049700	-0.69329700	1.25257400
H	-1.60309500	-1.72328100	1.25057200
H	-0.15767100	-0.67648300	1.24732200
H	-1.61417300	-0.18698100	2.14861100
C	-1.24688000	1.47357700	0.00082000
H	-1.59616200	2.00278000	-0.88470800
H	-1.59760900	2.00250100	0.88589800
H	-0.15419100	1.44499900	0.00144500

PC@O3; Eh = -657.2737439; Frequency = 36.2969

C	1.47413400	2.19942000	0.12785700
H	0.44628400	1.82798800	0.14057900
H	1.75691300	2.51188200	-0.87633300
H	1.60513600	3.01727400	0.83210300
I	-1.89303900	0.07191000	-0.07891200
C	1.65508500	-1.01082300	0.30121400

N	2.19046100	0.04802900	-0.26382400
O	2.37497400	1.17563600	0.59506700
O	2.55756800	0.18977300	-1.44031000
C	1.42341300	-2.15213200	-0.62540000
H	2.32858200	-2.39075500	-1.18752400
H	1.08969500	-3.02168500	-0.06311300
H	0.64270500	-1.87856300	-1.33993800
C	1.19344600	-1.03376400	1.71364400
H	1.58984600	-0.20012600	2.28355600
H	0.09959200	-0.98041000	1.71812000
H	1.50226300	-1.97251600	2.17970300

P@C3; Eh = -362.3335019; Frequency = 40.1823

C	0.96621000	-0.74722800	-1.25722400
H	2.05405300	-0.80080300	-1.28901100
H	0.61975400	-0.22649700	-2.15011200
H	0.56032800	-1.75640100	-1.25274700
C	0.54993500	0.00381000	-0.00000200
N	-0.97057700	0.02856300	0.00002500
O	-1.53791000	-1.06290700	-0.00000200
O	-1.54483700	1.11689100	0.00000400
C	0.96625800	-0.74688000	1.25741600
H	0.56040900	-1.75606700	1.25321400
H	2.05410400	-0.80040800	1.28920600
H	0.61979400	-0.22591900	2.15016800
C	1.07380200	1.42573200	-0.00021000

H	0.74356100	1.96884900	-0.88307800
H	0.74363000	1.96908300	0.88253900
H	2.16314000	1.38374700	-0.00024800

P@O3; Eh = -362.287239; Frequency = 43.9836

C	2.47404500	0.13253300	-0.00013800
H	2.64368400	-0.46935300	-0.88952700
H	2.64376300	-0.46947500	0.88915400
H	3.12248100	1.00408200	-0.00010500
C	-1.06160800	0.14853900	-0.00016300
N	0.16635700	-0.32776600	0.00003800
O	1.16509100	0.70752200	-0.00003200
O	0.54397500	-1.50075500	0.00028600
C	-2.12741500	-0.89311500	-0.00019800
H	-2.04421000	-1.53850500	0.87725200
H	-3.10721500	-0.42278700	-0.00479000
H	-2.03826300	-1.54396100	-0.87296400
C	-1.28654000	1.62264100	0.00015100
H	-0.84675700	2.09863400	0.87775400
H	-0.84527900	2.09923600	-0.87636200
H	-2.35612200	1.81876800	-0.00061900

[c-(CH₂)₂CNO₂]⁻ ; Eh = -321.2674228; Frequency = 140.9992

N	0.81267000	0.00000000	-0.09870500
O	1.41694400	1.10242500	0.08365800
O	1.41694300	-1.10242500	0.08365800

C	-0.47652400	0.00000000	-0.55996300
C	-1.53120300	-0.77079100	0.12421100
C	-1.53120300	0.77079100	0.12421100
H	-1.28446900	-1.24370100	1.07118100
H	-2.27863400	-1.29712100	-0.46035800
H	-2.27863400	1.29712100	-0.46035800
H	-1.28446900	1.24370000	1.07118100

RC@C4; Eh = -655.9850812; Frequency = 28.1968

C	-0.29837000	-0.39408800	0.00000200
H	-0.14577700	-1.46392300	0.00000400
H	0.09497400	0.08008500	-0.89140500
H	0.09497000	0.08008900	0.89140800
I	-2.42249300	-0.08417000	-0.00000200
N	2.37296800	0.81420400	0.00000300
O	2.16072500	1.40971400	1.10325400
O	2.16072300	1.40971500	-1.10324700
C	2.70934800	-0.50936500	0.00000200
C	3.84744400	-1.03758800	-0.77126400
C	3.84744600	-1.03758700	0.77126700
H	4.51536500	-0.32558700	-1.24741500
H	3.74982900	-1.98358200	-1.29300800
H	3.74982600	-1.98358000	1.29301400
H	4.51537300	-0.32558900	1.24741200

RC@O4; Eh = -655.9850876; Frequency = 27.7236

C	0.46983200	0.58187200	-0.42400600
H	-0.19518800	-0.26753200	-0.54226400
H	0.15537600	1.19652600	0.41069300
H	0.56535300	1.15521700	-1.33570900
I	2.41158100	-0.18924400	0.03258800
N	-2.40355600	0.73274800	0.12050700
O	-2.20954400	1.46189500	-0.90485400
O	-2.18596500	1.19846400	1.28339800
C	-2.72352700	-0.58437200	-0.03933300
C	-3.83812800	-1.22032400	0.68259300
C	-3.87368900	-1.02636600	-0.84720000
H	-4.50261900	-0.58245500	1.25815700
H	-3.71747600	-2.22238200	1.07913100
H	-3.77699900	-1.89718100	-1.48637500
H	-4.56019000	-0.26920200	-1.21500800

TS@C4; Eh = -655.9810893; Frequency = -343.3907

C	0.04984900	0.20184600	-0.00008700
H	-0.01760100	1.27628400	0.00001400
H	-0.19551500	-0.30702200	-0.91812500
H	-0.19559800	-0.30720600	0.91782800
I	2.36518500	-0.01649500	-0.00001400
N	-2.70391700	-0.85123400	0.00001500
O	-2.83657500	-1.45510800	1.10323600
O	-2.83708000	-1.45507600	-1.10316200
C	-2.27815800	0.45409100	-0.00005400

C	-2.91324600	1.53038500	-0.77113300
C	-2.91297900	1.53037400	0.77126200
H	-3.86506800	1.32744300	-1.25176800
H	-2.28648900	2.24862200	-1.29091400
H	-2.28603800	2.24860000	1.29083800
H	-3.86463400	1.32743500	1.25222800

TS@O4; Eh = -655.9937685; Frequency = -578.4961

C	-0.16110100	-0.01638100	0.58254700
H	0.08789900	-0.70146800	-0.20699500
H	-0.10975200	1.04175100	0.40960900
H	-0.44174300	-0.39463800	1.54571800
I	-2.61239600	-0.08301900	-0.13854700
N	2.40804400	0.49292000	0.22905000
O	1.68659800	-0.06216900	1.17751000
O	2.22404900	1.70597100	-0.05141700
C	3.24945400	-0.29642600	-0.45398600
C	4.63937500	-0.01698300	-0.81008900
C	4.24465400	-1.22919600	0.07268500
H	5.13516000	0.80954200	-0.31121500
H	4.98342700	-0.21656200	-1.81790200
H	4.32917700	-2.21846400	-0.36111600
H	4.49703600	-1.16712400	1.12586200

PC@C4; Eh = -656.0846083; Frequency = 46.5323

C	0.76831600	1.70718800	0.00000000
H	1.13220700	0.67604900	0.00000000
H	1.13506900	2.21805300	0.89140000
H	1.13506900	2.21805300	-0.89140000
I	1.02616400	-2.13592500	0.00000000
N	-1.30890700	3.03300600	0.00000000
O	-1.50689900	3.57746800	-1.08947900
O	-1.50689900	3.57746800	1.08947900
C	-0.73115500	1.66487200	0.00000000
C	-1.50689900	0.64316200	0.75903600
C	-1.50689900	0.64316200	-0.75903600
H	-2.40018400	0.97885100	1.26576700
H	-0.92805900	-0.14331700	1.22677100
H	-0.92805900	-0.14331700	-1.22677100
H	-2.40018400	0.97885100	-1.26576700

PC@O4; Eh = -656.0005335; Frequency = 18.6421

C	0.60010500	0.99434200	-0.07169700
H	0.65804000	1.65866300	-0.93162200
H	0.66318300	1.56587300	0.85017600
H	-0.32171600	0.41168500	-0.09559600
I	-3.03415100	-0.15308900	0.01760700
N	2.92699100	0.58375100	-0.10058400
O	1.64771800	0.00700600	-0.13265800
O	3.03697400	1.78599400	0.13463100
C	3.87687300	-0.28549800	-0.40225500

C	5.16788400	-0.52781800	0.23255400
C	4.11311700	-1.65084000	0.04760900
H	5.32106900	-0.15165700	1.23754300
H	6.05502300	-0.57441200	-0.38547500
H	4.32634700	-2.41276400	-0.69065200
H	3.59371400	-1.99503700	0.93349000

P@C4; Eh = -361.0978842; Frequency = 76.3736

C	-0.72489300	1.69668500	-0.00020500
H	-1.80379400	1.84675000	-0.00032200
H	-0.30396200	2.17338700	-0.88323100
H	-0.30412100	2.17353600	0.88281200
N	0.97962000	-0.13111900	0.00000300
O	1.27859900	-1.32476700	-0.00023300
O	1.78846500	0.79809300	0.00022200
C	-0.44990000	0.22534300	-0.00006300
C	-1.32853600	-0.73923300	-0.75017100
C	-1.32844900	-0.73904100	0.75045500
H	-0.82923300	-1.56362900	-1.23537500
H	-2.16659000	-0.29917600	-1.26988500
H	-2.16642700	-0.29885300	1.27017800
H	-0.82906800	-1.56331300	1.23579500

P@O4; Eh = -361.02129; Frequency = 53.6677

C	-2.48706500	-0.40159100	0.00509700
H	-2.72979300	0.08950100	-0.93555700

H	-2.74092000	0.24859500	0.83816200
H	-3.01452300	-1.34764900	0.08602200
N	-0.25943600	0.35729300	-0.06662300
O	-1.11285300	-0.79393500	0.04267500
O	-0.76757500	1.46350700	0.06077100
C	0.97295400	0.01646500	-0.36108200
C	2.27613900	0.48579800	0.08526200
C	1.89243000	-1.01896300	0.08384200
H	2.33914700	0.98536500	1.04429200
H	2.99416500	0.80782600	-0.65679500
H	2.37001300	-1.64342800	-0.65933900
H	1.71463600	-1.48808400	1.04330000
