

Supporting information for:

**Theoretical Investigation on the Reaction Mechanism of
Photocatalytic CO₂ Reduction over NaTaO₃ Modified with
Metal Cocatalysts (Ru, Rh, Ag)**

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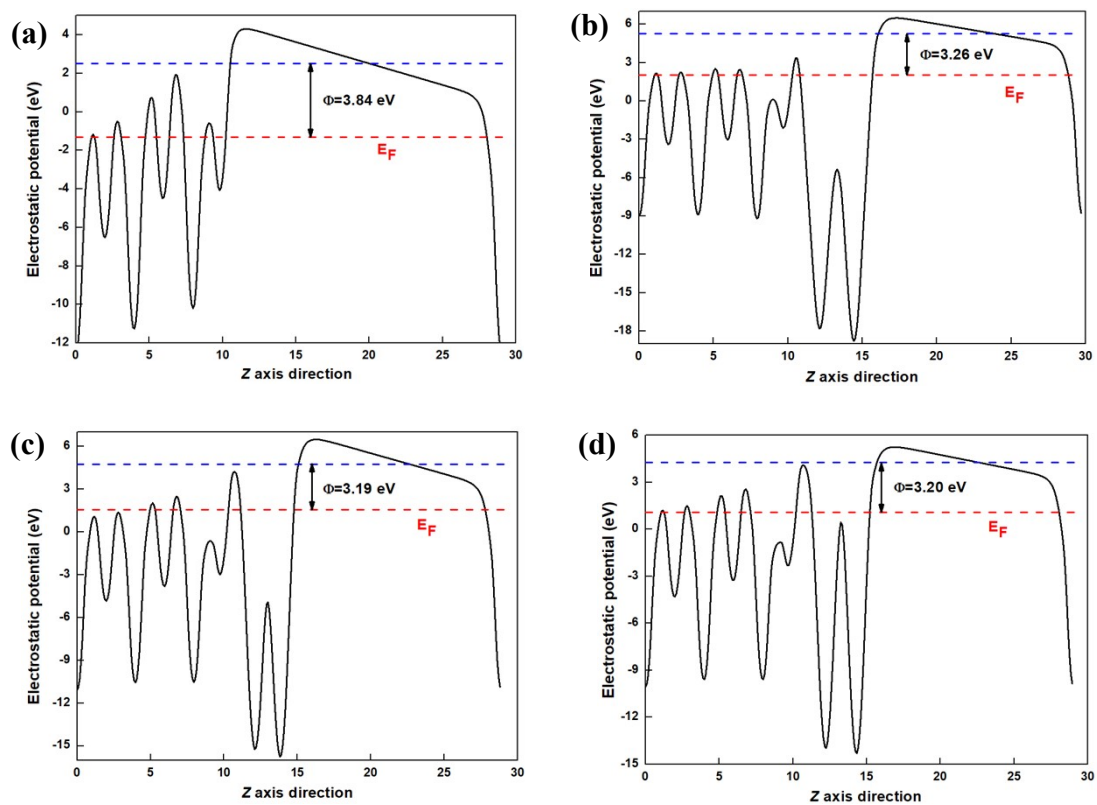


Figure S1. Electrostatic potentials (in eV) calculated for (a) clean $\text{NaTaO}_3(001)$ surface, (b) Ru@NaTaO_3 , (c) Rh@NaTaO_3 , and (d) Ag@NaTaO_3 . Blue and red dashed lines represent the vacuum level and the Fermi level, respectively.

The structural information of Ru@NaTaO₃

8.2384996414000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0431003571000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.7859992980999984

Ta	Na	O	Ru
12	12	36	24

Direct

0.2509500000000031	0.5000000000000000	0.0000000000000000
0.2509500000000031	0.0000000000000000	0.0000000000000000
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0.7509500000000031	0.5000000000000000	0.0000000000000000
0.7505700000000033	0.0000000000000000	0.1331699999999998
0.2505700000000033	0.5000000000000000	0.1331699999999998
0.2505700000000033	0.0000000000000000	0.1331699999999998
0.7505700000000033	0.5000000000000000	0.1331699999999998
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0.2408703880132113	0.5000098532987348	0.2655842111692551
0.7408661472515876	0.5000110955648263	0.2655866352768294
0.2397782154596228	0.0000206703178570	0.2673416336603446
0.0007599999999996	0.7500000000000000	0.0665800000000019
0.0007599999999996	0.2500000000000000	0.0665800000000019
0.5007599999999996	0.2500000000000000	0.0665800000000019
0.5007599999999996	0.7500000000000000	0.0665800000000019
0.5003799999999998	0.2500000000000000	0.1997500000000016
0.0003799999999998	0.7500000000000000	0.1997500000000016
0.0003799999999998	0.2500000000000000	0.1997500000000016
0.5003799999999998	0.7500000000000000	0.1997500000000016
0.4924033998758974	0.2561101711425804	0.3175708418141076
.0075915000232899	0.7438930769419425	0.3175668838238687
0.4924068935097286	0.7438935743104466	0.3175665881062266
.0075962026717219	0.2561104936985019	0.3175714028012101
0.2509500000000031	0.7500000000000000	0.0000000000000000
0.2509500000000031	0.2500000000000000	0.0000000000000000
0.7509500000000031	0.7500000000000000	0.0000000000000000
0.0009500000000031	0.0000000000000000	0.0000000000000000

0.7509500000000031	0.2500000000000000	0.0000000000000000
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0.2507599999999996	0.5000000000000000	0.0665800000000019
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0.5005700000000033	0.0000000000000000	0.1331699999999998
0.7505700000000033	0.2500000000000000	0.1331699999999998
0.2505700000000033	0.7500000000000000	0.1331699999999998
0.5005700000000033	0.5000000000000000	0.1331699999999998
0.2505700000000033	0.2500000000000000	0.1331699999999998
0.7505700000000033	0.7500000000000000	0.1331699999999998
0.0005700000000033	0.5000000000000000	0.1331699999999998
0.2503799999999998	0.5000000000000000	0.1997500000000016
0.7503799999999998	0.5000000000000000	0.1997500000000016
0.2503799999999998	0.0000000000000000	0.1997500000000016
0.7503799999999998	0.0000000000000000	0.1997500000000016
0.7521191357244249	0.2477515493218196	0.2661911910747902
0.0020580727332212	0.4999901517825021	0.2643607843717318
0.0024530416074598	0.0000076157511122	0.2669745046477709
0.2521178063339976	0.2477521088591306	0.2661911719274945
0.7521164583250713	0.7522558422035673	0.2661942350634476
0.2521133199110635	0.7522552014943633	0.2661945268504650
0.5024551304429390	0.0000069888625758	0.2669745015971614
0.5020598806369596	0.4999913824630278	0.2643610137342021
0.7515629932538100	0.0000111695017364	0.3347750668830481
0.2515617084928688	0.0000143814537868	0.3347747221274825
0.2533236264010024	0.4999900996466385	0.3292019454602023
0.7533279439169439	0.4999883057353274	0.3292000782710240
0.7498366222190255	0.8382445549996773	0.3943337697144782
0.2498542310928211	0.1617714951754294	0.3943341587890044
0.2498363828624870	0.8382448532808264	0.3943334936870530

0.7498551136302549	0.1617717162344667	0.3943350379065879
0.7505753609913530	0.5000102665189132	0.3941035939753242
0.2505725068734237	0.5000070556600213	0.3941033415400679
0.4999917680380230	0.0000059082571314	0.4207027156152714
0.5003939532895246	0.3314366790098299	0.4204858185716696
0.0003958437891380	0.3314350803888035	0.4204862169950512
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0.2501751702859707	0.3331330333000094	0.4728598369229678
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0.0000594018343298	0.5000079185523097	0.4965916355936327
0.5001258277259103	0.8327223681140655	0.4965975712344461
0.0001476099449995	0.1673246995060148	0.4965950946678613
0.0001261533537026	0.8327202340377997	0.4965976378399167

The structural information of *CO₂

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0.0000000000000000	8.0431003571000002	0.0000000000000000		
0.0000000000000000	0.0000000000000000	29.7859992980999984		
Ta	Na	O	Ru	C
12	12	38	24	1
Direct				
0.2509500090000003	0.5000000000000000	0.0000000000000000		
0.2509500090000003	0.0000000000000000	0.0000000000000000		
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0.75094997899999978	0.5000000000000000	0.0000000000000000		
0.7505699989999997	0.0000000000000000	0.1331699939999993		

0.2505699989999997	0.5000000000000000	0.1331699939999993
0.2505699989999997	0.0000000000000000	0.1331699939999993
0.7505699989999997	0.5000000000000000	0.1331699939999993
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0.2392303607803541	0.0007735550709206	0.2673511414491484
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0.0007599999999996	0.2500000000000000	0.0665799980000017
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0.5005699989999997	0.5000000000000000	0.1331699939999993
0.2505699989999997	0.2500000000000000	0.1331699939999993
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0.7503799799999982	0.5000000000000000	0.1997500060000021
0.2503800089999970	0.0000000000000000	0.1997500060000021
0.7503799799999982	0.0000000000000000	0.1997500060000021
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0.0018796993508173	0.0010240687715721	0.2672202279229225
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0.2495668671587161	0.4965650720600427	0.3291867564773749
0.7568764892668228	0.5025314206601522	0.3291394086434395
0.3629910050855658	0.4176850863820709	0.5598806114589404
0.1249267663338784	0.2695966824358703	0.5598137312529478
0.7486648307344822	0.8377838987303137	0.3947993348831835
0.2463370202089419	0.1585345537240276	0.3944577285732333
0.2489775766518168	0.8387763228508598	0.3952788564449435
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0.7492316064156517	0.3336754974123353	0.4736979784578768
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0.0010477985620067	0.1693951050330748	0.5004194692874464
0.0003444695303061	0.8301382315596634	0.4973940440102273
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The structural information of *COOH

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0.0000000000000000	8.0431003571000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.7859992980999984

Ta	Na	O	Ru	C	H
12	12	38	24	1	1

Direct

0.2509500000000031	0.5000000000000000	0.0000000000000000
0.2509500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.5000000000000000	0.0000000000000000
0.7505700000000033	0.0000000000000000	0.1331699999999998
0.2505700000000033	0.5000000000000000	0.1331699999999998
0.2505700000000033	0.0000000000000000	0.1331699999999998
0.7505700000000033	0.5000000000000000	0.1331699999999998
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0.7403166367406413	0.5001146528502870	0.2655903754962244
0.2395751804073041	0.0001676083422871	0.2674851822877581
0.0007599999999996	0.7500000000000000	0.0665800000000019
0.0007599999999996	0.2500000000000000	0.0665800000000019
0.5007599999999996	0.2500000000000000	0.0665800000000019

0.5007599999999996	0.7500000000000000	0.0665800000000019
0.5003799999999998	0.2500000000000000	0.1997500000000016
0.0003799999999998	0.7500000000000000	0.1997500000000016
0.0003799999999998	0.2500000000000000	0.1997500000000016
0.5003799999999998	0.7500000000000000	0.1997500000000016
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0.9918128316238711	0.7435195533925022	0.3178342608891966
0.4918228512290829	0.7450021028810738	0.3176833534439941
0.9916710113214009	0.2572494314607627	0.3177232126959332
0.2509500000000031	0.7500000000000000	0.0000000000000000
0.2509500000000031	0.2500000000000000	0.0000000000000000
0.7509500000000031	0.7500000000000000	0.0000000000000000
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0.7509500000000031	0.2500000000000000	0.0000000000000000
0.0009500000000031	0.5000000000000000	0.0000000000000000
0.5009500000000031	0.5000000000000000	0.0000000000000000
0.5009500000000031	0.0000000000000000	0.0000000000000000
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0.2507599999999996	0.0000000000000000	0.0665800000000019
0.0005700000000033	0.0000000000000000	0.1331699999999998
0.5005700000000033	0.0000000000000000	0.1331699999999998
0.7505700000000033	0.2500000000000000	0.1331699999999998
0.2505700000000033	0.7500000000000000	0.1331699999999998
0.5005700000000033	0.5000000000000000	0.1331699999999998
0.2505700000000033	0.2500000000000000	0.1331699999999998
0.7505700000000033	0.7500000000000000	0.1331699999999998
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0.2503799999999998	0.5000000000000000	0.1997500000000016
0.7503799999999998	0.5000000000000000	0.1997500000000016
0.2503799999999998	0.0000000000000000	0.1997500000000016
0.7503799999999998	0.0000000000000000	0.1997500000000016
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0.2519022087491744	0.2480416578229856	0.2660144620882985
0.7517552366246130	0.7521687686808038	0.2662897097000443
0.2517157356961531	0.7521314556511450	0.2663084262830462
0.5021909564142901	-0.0000491487510684	0.2665101885666959
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0.7483929464846950	0.0009715800682828	0.3346258119291691
0.2548692531092865	0.0011665623880352	0.3345870614462200
0.2508506982498231	0.4991474434707805	0.3292422996430435
0.7554379332448317	0.4992737541113986	0.3292140202263527
0.4991876262999138	0.7518119871450546	0.5674107715994496
0.4991025656271579	0.5040389377910164	0.5996363755443382
0.7499478713062071	0.8368443841662359	0.3951662839506027
0.2477402749085850	0.1599167148839396	0.3946844638527193
0.2492153660441770	0.8367854575293359	0.3951650225677624
0.7512661718216275	0.1598547826201360	0.3946965383346549
0.7482817524883580	0.4989077525766144	0.3941062211190530
0.2525836131153454	0.4989582683753869	0.3941413547315871
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0.5002130943798403	0.3284212076560346	0.4191085957156078
0.0001101973542655	0.3308411514990396	0.4211035263440532
0.0000750489071699	0.6663868084226309	0.4209100694423137
0.9997138853890881	-0.0018200370541752	0.4215227490858623
0.5002252234707210	0.6658845560806870	0.4200678943814836
0.2511879372007992	0.3321360054906057	0.4731027454426032
0.7486829564978388	0.3321166332042491	0.4731030772210091
0.2524606526963419	-0.0018880077941102	0.4733861391317369
0.7503957191371893	0.6662607200916975	0.4725605003731417
0.7471964116218263	-0.0019263211882332	0.4733884048058963
0.2494687408128076	0.6662637754403113	0.4725317052785297
0.4999577626226707	0.5019027882838503	0.4982915659480346
0.4998443548291242	0.1682267616435176	0.4969596457424039
-0.0001101034645576	0.4981470738220835	0.4964188652680870
0.4998968093109754	0.8331832348973344	0.4992351389405204
-0.0001060364496334	0.1657486961075670	0.4964085973475675

-0.0001219210564489	0.8313264347457608	0.4966230894610684
0.4992615528301724	0.5949572471639767	0.5615194299826032
0.4992541019880022	0.3874505201309366	0.5899597234292470

The structural information of *CO

8.2384996414000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0431003571000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.7859992980999984

Ta	Na	O	Ru	C
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12	12	37	24	1
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Direct

0.2509500000000031	0.5000000000000000	0.0000000000000000
0.2509500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.5000000000000000	0.0000000000000000
0.7505700000000033	0.0000000000000000	0.1331699999999998
0.2505700000000033	0.5000000000000000	0.1331699999999998
0.2505700000000033	0.0000000000000000	0.1331699999999998
0.7505700000000033	0.5000000000000000	0.1331699999999998
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0.7404724420878620	0.4999978649645936	0.2656058713319636
0.2399599573839306	0.0000036700810515	0.2675094466194058
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0.0007599999999996	0.2500000000000000	0.0665800000000019
0.5007599999999996	0.2500000000000000	0.0665800000000019
0.5007599999999996	0.7500000000000000	0.0665800000000019
0.5003799999999998	0.2500000000000000	0.1997500000000016
0.0003799999999998	0.7500000000000000	0.1997500000000016
0.0003799999999998	0.2500000000000000	0.1997500000000016
0.5003799999999998	0.7500000000000000	0.1997500000000016
0.4919104334332351	0.2546805989815326	0.3174368819701847
0.9920465946223691	0.7431901785970881	0.3177480693709931
0.4919099115720699	0.7453233941662903	0.3174409377734402
0.9920499764507044	0.2568116437056419	0.3177446259907889
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0.2509500000000031	0.2500000000000000	0.0000000000000000
0.7509500000000031	0.7500000000000000	0.0000000000000000
0.0009500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.2500000000000000	0.0000000000000000
0.0009500000000031	0.5000000000000000	0.0000000000000000
0.5009500000000031	0.5000000000000000	0.0000000000000000
0.5009500000000031	0.0000000000000000	0.0000000000000000
0.7507599999999996	0.0000000000000000	0.0665800000000019
0.7507599999999996	0.5000000000000000	0.0665800000000019
0.2507599999999996	0.5000000000000000	0.0665800000000019
0.2507599999999996	0.0000000000000000	0.0665800000000019
0.0005700000000033	0.0000000000000000	0.1331699999999998
0.5005700000000033	0.0000000000000000	0.1331699999999998
0.7505700000000033	0.2500000000000000	0.1331699999999998
0.2505700000000033	0.7500000000000000	0.1331699999999998
0.5005700000000033	0.5000000000000000	0.1331699999999998
0.2505700000000033	0.2500000000000000	0.1331699999999998
0.7505700000000033	0.7500000000000000	0.1331699999999998
0.0005700000000033	0.5000000000000000	0.1331699999999998
0.2503799999999998	0.5000000000000000	0.1997500000000016
0.7503799999999998	0.5000000000000000	0.1997500000000016
0.2503799999999998	0.0000000000000000	0.1997500000000016
0.7503799999999998	0.0000000000000000	0.1997500000000016
0.7519492896202040	0.2478922673769452	0.2661867922634530
0.0018712669527606	0.5000022257699027	0.2641940936309708
0.0025038571887195	0.0000018485246571	0.2676014119621676
0.2518924749937093	0.2479404683588667	0.2661631918728783
0.7519529410323591	0.7521108427651716	0.2661893045096604
0.2518902536889598	0.7520661627100300	0.2661662728890047
0.5023124853036148	-0.0000022099748987	0.2662223082644891
0.5019802619396285	0.5000052297027215	0.2645802900865142
0.7466083502289669	0.0000186353003898	0.3346321774646698
0.2568504124357920	0.0000215439435696	0.3345526329609901
0.2515129975600343	0.4999956665005050	0.3292510735851563
0.7546757691983498	0.4999985961919325	0.3292426376949670

0.4988507121469268	0.5009872335539696	0.6020499225904444
0.7507075921601724	0.8381368129858674	0.3948722141929275
0.2487704296808574	0.1619505947444629	0.3948610992085445
0.2487697850281554	0.8380673363434504	0.3948610856458408
0.7507093748499837	0.1618976064418311	0.3948730899785516
0.7482448505520460	0.5000178327318882	0.3941281249754471
0.2528437577090334	0.5000125957596803	0.3941506644452258
0.4998635451466416	0.0000047782242254	0.4211470061345007
0.5003411042626760	0.3315996071624056	0.4196096372975525
0.0002456844027074	0.3319975419006415	0.4208506588581116
0.0002428495577897	0.6680274285316452	0.4208506827624960
0.9998961516267020	0.0000127067686611	0.4207031093078823
0.5003407838063432	0.6684246733079776	0.4196071969163950
0.2502117118504614	0.3321842594518327	0.4727216941134077
0.7499654630848762	0.3321857388733999	0.4727425255711551
0.2488627206660637	0.0000248747136546	0.4733321933961433
0.7499650037026061	0.6678692051921857	0.4727427129380202
0.7511638628114147	0.0000254575299368	0.4733445002075927
0.2502086965313847	0.6678608063271940	0.4727209758055673
0.5000639070104388	0.5000363619515249	0.4997756933094404
0.5000513856976443	0.1652400387204254	0.4963301721318085
0.0000149458401279	0.5000140536157575	0.4962058653775304
0.5000474722010779	0.8348228779961747	0.4963301581065150
0.0000572838967623	0.1679788757800901	0.4966892394633784
0.0000596870976529	0.8320518630939567	0.4966903017812974
0.4993281183625290	0.5005804072148291	0.5626907941807010

The structural information of *COH

8.2384996414000007	0.0000000000000000	0.0000000000000000			
0.0000000000000000	8.0431003571000002	0.0000000000000000			
0.0000000000000000	0.0000000000000000	29.7859992980999984			
Ta	Na	O	Ru	C	H
12	12	37	24	1	1
Direct					
0.2509500090000003	0.5000000000000000	0.0000000000000000			
0.2509500090000003	0.0000000000000000	0.0000000000000000			

0.7509499789999978	0.0000000000000000	0.0000000000000000
0.7509499789999978	0.5000000000000000	0.0000000000000000
0.7505699989999997	0.0000000000000000	0.1331699939999993
0.2505699989999997	0.5000000000000000	0.1331699939999993
0.2505699989999997	0.0000000000000000	0.1331699939999993
0.7505699989999997	0.5000000000000000	0.1331699939999993
0.7389409089520923	0.0007714537104722	0.2673140969789511
0.2400219978623415	0.5004059078294106	0.2655458672251003
0.7402246947252094	0.5004355361773914	0.2655867043405904
0.2391279648199304	0.0001062999009404	0.2672741649611195
0.0007599999999996	0.7500000000000000	0.0665799980000017
0.0007599999999996	0.2500000000000000	0.0665799980000017
0.5007600189999977	0.2500000000000000	0.0665799980000017
0.5007600189999977	0.7500000000000000	0.0665799980000017
0.5003799799999982	0.2500000000000000	0.1997500060000021
0.0003799999999998	0.7500000000000000	0.1997500060000021
0.0003799999999998	0.2500000000000000	0.1997500060000021
0.5003799799999982	0.7500000000000000	0.1997500060000021
0.4914801289389424	0.2574631402409886	0.3178937057375895
0.9910522662945622	0.7444786385342924	0.3176007329484672
0.4919178394168066	0.7457068610869055	0.3172938848752185
0.9918982099816515	0.2575807574726490	0.3177159145942826
0.2509500090000003	0.7500000000000000	0.0000000000000000
0.2509500090000003	0.2500000000000000	0.0000000000000000
0.7509499789999978	0.7500000000000000	0.0000000000000000
0.00095000000000031	0.0000000000000000	0.0000000000000000
0.7509499789999978	0.2500000000000000	0.0000000000000000
0.00095000000000031	0.5000000000000000	0.0000000000000000
0.5009499789999978	0.5000000000000000	0.0000000000000000
0.5009499789999978	0.0000000000000000	0.0000000000000000
0.7507600189999977	0.0000000000000000	0.0665799980000017
0.7507600189999977	0.5000000000000000	0.0665799980000017
0.25075998900000023	0.5000000000000000	0.0665799980000017
0.25075998900000023	0.0000000000000000	0.0665799980000017
0.00057000000000033	0.0000000000000000	0.1331699939999993

0.5005699989999997	0.0000000000000000	0.1331699939999993
0.7505699989999997	0.2500000000000000	0.1331699939999993
0.2505699989999997	0.7500000000000000	0.1331699939999993
0.5005699989999997	0.5000000000000000	0.1331699939999993
0.2505699989999997	0.2500000000000000	0.1331699939999993
0.7505699989999997	0.7500000000000000	0.1331699939999993
0.00057000000000033	0.5000000000000000	0.1331699939999993
0.2503800089999970	0.5000000000000000	0.1997500060000021
0.7503799799999982	0.5000000000000000	0.1997500060000021
0.2503800089999970	0.0000000000000000	0.1997500060000021
0.7503799799999982	0.0000000000000000	0.1997500060000021
0.7518851074165839	0.2482151243947875	0.2660227233216387
0.0014593532658155	0.5007011843377333	0.2642863013008970
0.0017066004438354	-0.0003866287661705	0.2671081364006266
0.2508268013808267	0.2475212369079298	0.2663405333172638
0.7507191464426559	0.7525495286889845	0.2663898983822912
0.2519181781467033	0.7519311695826760	0.2659187389378704
0.5018020839767596	0.0006353077165285	0.2667021690268823
0.5017598516732834	0.4997591509332747	0.2645604960085005
0.7486172365921826	0.0021020050756331	0.3347359171353012
0.2519903728605051	-0.0040006097630276	0.3346148964561065
0.2521226913042325	0.4995097143748274	0.3291338937025201
0.7541239557039195	0.4995380469283363	0.3293059460956125
0.6811478607030138	0.3309685617168301	0.5779213807915234
0.7498218571195022	0.8354693167706455	0.3954324797506605
0.2496686938901888	0.1597005623602319	0.3944672263378715
0.2477234682359580	0.8360282466973296	0.3938675299332026
0.7500211105463365	0.1570515708396826	0.3942476693410532
0.7478111529983745	0.4966003485157787	0.3941939902501425
0.2515210761801389	0.4972876242600599	0.3939989764410695
0.4978643727096579	-0.0029124137292960	0.4200511819650756
0.5026297184299221	0.3293647074045489	0.4212897853023248
-0.0011411057895256	0.3294806255491688	0.4209734186048062
0.0026198635218337	0.6653632584940807	0.4206025605629544
0.0008280743119776	-0.0028260062530821	0.4209233370061953

0.4967038890521639	0.6671820584184482	0.4196650483417140
0.2489926477372001	0.3306775562262922	0.4721026224610211
0.7514897456514738	0.3315194451273201	0.4747635293309091
0.2502694345729912	-0.0046421906462026	0.4735551577275523
0.7497773783920723	0.6654357610388384	0.4716944511553559
0.7499254800543144	-0.0020556851721882	0.4723764547452432
0.2501391426911604	0.6670557757643198	0.4735691710600806
0.4957735558038361	0.4952239968792778	0.4983329335213627
0.4979025667911994	0.1648357861376478	0.4984073901777553
0.0032765036063203	0.4994170858025589	0.4965813068772059
0.5017087293405055	0.8302507823689221	0.4960916963554357
0.0043653132372178	0.1623789170780736	0.4967523551540783
0.9965392379842510	0.8299486968307028	0.4962684324547536
0.6298005208463872	0.3374849020483814	0.5350321535128920
0.7714301130798695	0.2510829161527384	0.5796059312489541

The structural information of *C

8.2384996414000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0431003571000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.7859992980999984

Ta	Na	O	Ru	C
----	----	---	----	---

12	12	36	24	1
----	----	----	----	---

Direct

0.2509500090000003	0.5000000000000000	0.0000000000000000
0.2509500090000003	0.0000000000000000	0.0000000000000000
0.7509499789999978	0.0000000000000000	0.0000000000000000
0.7509499789999978	0.5000000000000000	0.0000000000000000
0.7505699989999997	0.0000000000000000	0.1331699939999993
0.2505699989999997	0.5000000000000000	0.1331699939999993
0.2505699989999997	0.0000000000000000	0.1331699939999993
0.7505699989999997	0.5000000000000000	0.1331699939999993
0.7399267388384140	-0.0005141327988818	0.2672379935963392
0.2409177751247296	0.4992722621867203	0.2656586641825727
0.7408115205432108	0.4993795461450762	0.2654995031628493
0.2403479370535780	0.9991339404296097	0.2674508175481539
0.0007599999999996	0.7500000000000000	0.0665799980000017

0.0007599999999996	0.2500000000000000	0.0665799980000017
0.5007600189999977	0.2500000000000000	0.0665799980000017
0.5007600189999977	0.7500000000000000	0.0665799980000017
0.5003799799999982	0.2500000000000000	0.1997500060000021
0.0003799999999998	0.7500000000000000	0.1997500060000021
0.0003799999999998	0.2500000000000000	0.1997500060000021
0.5003799799999982	0.7500000000000000	0.1997500060000021
0.4923845098672556	0.2542344529853126	0.3175591867200710
0.9929715491051253	0.7423271607091421	0.3176898490965043
0.4919569902572118	0.7428017379661508	0.3176344497606091
0.9935702366423128	0.2556220229343080	0.3173467219456397
0.2509500090000003	0.7500000000000000	0.0000000000000000
0.2509500090000003	0.2500000000000000	0.0000000000000000
0.7509499789999978	0.7500000000000000	0.0000000000000000
0.0009500000000031	0.0000000000000000	0.0000000000000000
0.7509499789999978	0.2500000000000000	0.0000000000000000
0.0009500000000031	0.5000000000000000	0.0000000000000000
0.5009499789999978	0.5000000000000000	0.0000000000000000
0.5009499789999978	0.0000000000000000	0.0000000000000000
0.7507600189999977	0.0000000000000000	0.0665799980000017
0.7507600189999977	0.5000000000000000	0.0665799980000017
0.2507599890000023	0.5000000000000000	0.0665799980000017
0.2507599890000023	0.0000000000000000	0.0665799980000017
0.0005700000000033	0.0000000000000000	0.1331699939999993
0.5005699989999997	0.0000000000000000	0.1331699939999993
0.7505699989999997	0.2500000000000000	0.1331699939999993
0.2505699989999997	0.7500000000000000	0.1331699939999993
0.5005699989999997	0.5000000000000000	0.1331699939999993
0.2505699989999997	0.2500000000000000	0.1331699939999993
0.7505699989999997	0.7500000000000000	0.1331699939999993
0.0005700000000033	0.5000000000000000	0.1331699939999993
0.2503800089999970	0.5000000000000000	0.1997500060000021
0.7503799799999982	0.5000000000000000	0.1997500060000021
0.2503800089999970	0.0000000000000000	0.1997500060000021
0.7503799799999982	0.0000000000000000	0.1997500060000021

0.7521927081792528	0.2476705901074436	0.2660100016262690
0.0021964766057561	0.4992665299658430	0.2643823057762971
0.0029901809032036	0.9999232310184063	0.2673020938377422
0.2526476750669905	0.2475712108674022	0.2663957755763294
0.7527713290254631	0.7522065391924890	0.2662357978677201
0.2521275417852509	0.7518335753761296	0.2660625356704226
0.5028063146443768	0.9993887250349304	0.2665985951270688
0.5020877838468067	0.4997934466233372	0.2644273315185084
0.7498491009896074	0.0023507035837118	0.3346819049591484
0.2551343478096812	-0.0011917561250249	0.3347325059484754
0.2525341288345839	0.5012295648915426	0.3293471908125870
0.7531712734760168	0.5000956254233568	0.3290594219174439
0.7494924280462040	0.8386024324679157	0.3943986277287680
0.2498684942528940	0.1628929302243532	0.3952116243385934
0.2493320112011484	0.8404462853609942	0.3948853520110799
0.7519123422203230	0.1628138158898620	0.3937866730711505
0.7491066932668176	0.5026169952780251	0.3938065249131720
0.2530450785642993	0.5041693920059407	0.3944221897431205
0.5024517794072173	0.0014410817861824	0.4205295844599089
0.5040297919906133	0.3327804034496947	0.4200103030875760
-0.0023596106551422	0.3329788227822254	0.4201613351710332
-0.0009619440343777	0.6694158301587414	0.4208019247624564
-0.0013280020723535	0.0010688472169021	0.4206913096502438
0.4987413378547321	0.6696158344460384	0.4198085301545721
0.2491597974962093	0.3334919638196921	0.4711896092905848
0.7514162139298378	0.3308522516900859	0.4734571932570914
0.2490899327644364	0.0027153726752048	0.4719966360024499
0.7490193414001293	0.6676155891763920	0.4722884280313542
0.7502452072177871	0.0037615321501376	0.4735606742762399
0.2479573257896853	0.6681652415782663	0.4747885045229942
0.5031633804935772	0.4948033134631212	0.4991012824845981
0.4984687515472569	0.1695398593782460	0.4963081597213770
-0.0032486276104012	0.4998271491527064	0.4962501346801740
0.5014367735661397	0.8440815540048794	0.4997317812972843
0.0029443593419044	0.1690221993985752	0.4962522267726033

-0.0045115069465982 0.8361099304102235 0.4966015691325971
0.3880972678481601 0.6661644823639288 0.5299975539428400

The structural information of *CH

8.2384996414000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 8.0431003571000002 0.0000000000000000
0.0000000000000000 0.0000000000000000 29.7859992980999984

Ta Na O Ru C H
12 12 36 24 1 1

Direct

0.2509500000000031 0.5000000000000000 0.0000000000000000
0.2509500000000031 0.0000000000000000 0.0000000000000000
0.7509500000000031 0.0000000000000000 0.0000000000000000
0.7509500000000031 0.5000000000000000 0.0000000000000000
0.7505700000000033 0.0000000000000000 0.1331699999999998
0.2505700000000033 0.5000000000000000 0.1331699999999998
0.2505700000000033 0.0000000000000000 0.1331699999999998
0.7505700000000033 0.5000000000000000 0.1331699999999998
0.7389905142283120 -0.0000064552402730 0.2674575048968936
0.2398575546130810 0.4999975177120917 0.2655380657329598
0.7403278423444736 0.4999977045508330 0.2655552313708632
0.2396799876592856 -0.0000205754179691 0.2675130278690196
0.0007599999999996 0.7500000000000000 0.0665800000000019
0.0007599999999996 0.2500000000000000 0.0665800000000019
0.5007599999999996 0.2500000000000000 0.0665800000000019
0.5007599999999996 0.7500000000000000 0.0665800000000019
0.5003799999999998 0.2500000000000000 0.1997500000000016
0.0003799999999998 0.7500000000000000 0.1997500000000016
0.0003799999999998 0.2500000000000000 0.1997500000000016
0.5003799999999998 0.7500000000000000 0.1997500000000016
0.4917080375224221 0.2537451528642654 0.3174370285442145
0.9916726307346927 0.7424312365782321 0.3177711993591025
0.4916992755342361 0.7462887431924000 0.3174276803360495
0.9916791161652222 0.2575475333985037 0.3177713779710191
0.2509500000000031 0.7500000000000000 0.0000000000000000
0.2509500000000031 0.2500000000000000 0.0000000000000000

0.7509500000000031	0.7500000000000000	0.0000000000000000
0.0009500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.2500000000000000	0.0000000000000000
0.0009500000000031	0.5000000000000000	0.0000000000000000
0.5009500000000031	0.5000000000000000	0.0000000000000000
0.5009500000000031	0.0000000000000000	0.0000000000000000
0.7507599999999996	0.0000000000000000	0.0665800000000019
0.7507599999999996	0.5000000000000000	0.0665800000000019
0.2507599999999996	0.5000000000000000	0.0665800000000019
0.2507599999999996	0.0000000000000000	0.0665800000000019
0.0005700000000033	0.0000000000000000	0.1331699999999998
0.5005700000000033	0.0000000000000000	0.1331699999999998
0.7505700000000033	0.2500000000000000	0.1331699999999998
0.2505700000000033	0.7500000000000000	0.1331699999999998
0.5005700000000033	0.5000000000000000	0.1331699999999998
0.2505700000000033	0.2500000000000000	0.1331699999999998
0.7505700000000033	0.7500000000000000	0.1331699999999998
0.0005700000000033	0.5000000000000000	0.1331699999999998
0.2503799999999998	0.5000000000000000	0.1997500000000016
0.7503799999999998	0.5000000000000000	0.1997500000000016
0.2503799999999998	0.0000000000000000	0.1997500000000016
0.7503799999999998	0.0000000000000000	0.1997500000000016
0.7515524030135924	0.2478173332365781	0.2661810920183572
0.0016985244123160	0.4999962487733211	0.2638467322195791
0.0023032710531388	-0.0000016571013978	0.2676776663303601
0.2517745909413925	0.2478725158865154	0.2661640405325617
0.7515464382639747	0.7521810890610456	0.2661676684377250
0.2517838514681192	0.7521187268392691	0.2661486837602469
0.5020965421289117	0.0000045548404448	0.2661479411440364
0.5018905928865389	0.4999901554101422	0.2649226566201758
0.7454916387362455	-0.0000617477570529	0.3347132912234693
0.2574304762817173	-0.0000692715403432	0.3346157989038333
0.2492479847784687	0.5000474732222425	0.3292084033317185
0.7572955121923642	0.5000472013831927	0.3291574545532382
0.7503330489401739	0.8380672672191629	0.3949476073703148

0.2487323161699472	0.1619906418554828	0.3949601231415901
0.2487027320641107	0.8380050783392794	0.3949504056198783
0.7503005544838687	0.1619380955634887	0.3949591398809391
0.7471840207841276	0.4999955136007492	0.3939577219685526
0.2533532834524058	0.4999983229841187	0.3940243633705849
0.4996737420105052	0.0000289043655055	0.4215020699320984
0.5002338885411695	0.3325397419107061	0.4195690206137488
-0.0000790355357103	0.3319885567516425	0.4209881276673497
-0.0000790213575280	0.6680583100336802	0.4209964679902947
0.9996565306413753	0.0000192154991360	0.4206431502058844
0.5002331648196929	0.6675270970931109	0.4195365539362018
0.2512810136361942	0.3325116868009728	0.4725715644949112
0.7483951177897290	0.3326099067472271	0.4726624250316385
0.2477993620994215	-0.0000377655010934	0.4731669330144989
0.7483563303773377	0.6672895928355729	0.4726806718043889
0.7517966638339120	-0.0000325254224459	0.4732129657388735
0.2513043640969617	0.6673882900832120	0.4725913697276443
0.4996045640521617	0.4998559495133782	0.5040457046932119
0.4998247628787791	0.1635745124556722	0.4964824660824744
-0.0001831111747857	0.5000215319300939	0.4955882099405895
0.4998312935217763	0.8360909740278961	0.4964195017797901
-0.0001932378746720	0.1682511194456399	0.4965831299274038
-0.0001790263151560	0.8317797573986601	0.4965846095273697
0.4981415178697153	0.4962041695371825	0.5618582397609089
0.4965213025159798	0.4931570029825167	0.5986640182102014

The structural information of *CH₂

8.2384996414000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0431003571000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.7859992980999984

Ta	Na	O	Ru	C	H
12	12	36	24	1	2

Direct

0.25095000000000031	0.5000000000000000	0.0000000000000000
0.25095000000000031	0.0000000000000000	0.0000000000000000
0.75095000000000031	0.0000000000000000	0.0000000000000000

0.7509500000000031	0.5000000000000000	0.0000000000000000
0.7505700000000033	0.0000000000000000	0.1331699999999998
0.2505700000000033	0.5000000000000000	0.1331699999999998
0.2505700000000033	0.0000000000000000	0.1331699999999998
0.7505700000000033	0.5000000000000000	0.1331699999999998
0.7392035763207034	0.0000081173736590	0.2675048191623028
0.2398546685011433	0.5000126270008013	0.2655643570511294
0.7405107320860237	0.5000045894751316	0.2655943354159613
0.2396992983756460	0.0000132662909182	0.2675493653517970
0.0007599999999996	0.7500000000000000	0.0665800000000019
0.0007599999999996	0.2500000000000000	0.0665800000000019
0.5007599999999996	0.2500000000000000	0.0665800000000019
0.5007599999999996	0.7500000000000000	0.0665800000000019
0.5003799999999998	0.2500000000000000	0.1997500000000016
0.0003799999999998	0.7500000000000000	0.1997500000000016
0.0003799999999998	0.2500000000000000	0.1997500000000016
0.5003799999999998	0.7500000000000000	0.1997500000000016
0.4917438818372144	0.2542476553094746	0.3174716678589813
0.9917973118480997	0.7425010870506622	0.3179484307932946
0.4917654327512385	0.7458231686156013	0.3174116536846456
0.9917934941901080	0.2574751862119295	0.3179498755781036
0.2509500000000031	0.7500000000000000	0.0000000000000000
0.2509500000000031	0.2500000000000000	0.0000000000000000
0.7509500000000031	0.7500000000000000	0.0000000000000000
0.0009500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.2500000000000000	0.0000000000000000
0.0009500000000031	0.5000000000000000	0.0000000000000000
0.5009500000000031	0.5000000000000000	0.0000000000000000
0.5009500000000031	0.0000000000000000	0.0000000000000000
0.7507599999999996	0.0000000000000000	0.0665800000000019
0.7507599999999996	0.5000000000000000	0.0665800000000019
0.2507599999999996	0.5000000000000000	0.0665800000000019
0.2507599999999996	0.0000000000000000	0.0665800000000019
0.0005700000000033	0.0000000000000000	0.1331699999999998
0.5005700000000033	0.0000000000000000	0.1331699999999998

0.7505700000000033	0.2500000000000000	0.1331699999999998
0.2505700000000033	0.7500000000000000	0.1331699999999998
0.5005700000000033	0.5000000000000000	0.1331699999999998
0.2505700000000033	0.2500000000000000	0.1331699999999998
0.7505700000000033	0.7500000000000000	0.1331699999999998
0.0005700000000033	0.5000000000000000	0.1331699999999998
0.2503799999999998	0.5000000000000000	0.1997500000000016
0.7503799999999998	0.5000000000000000	0.1997500000000016
0.2503799999999998	0.0000000000000000	0.1997500000000016
0.7503799999999998	0.0000000000000000	0.1997500000000016
0.7516261862389920	0.2478743493902327	0.2661992930812755
0.0017637383809055	0.5000045514268495	0.2637597030771002
0.0024016717212423	0.0000093209779179	0.2675443428792320
0.2520187292746765	0.2479353546374645	0.2661839705765088
0.7516205902729676	0.7521588060577061	0.2661886276599186
0.2520141928481300	0.7520982405325680	0.2661711598350351
0.5022571567809678	-0.0000006890759461	0.2663996283108673
0.5020122594912286	0.5000089414520525	0.2650009942198249
0.7469827203648869	0.0000439958686873	0.3347609440507495
0.2562106639174389	0.0000431194591727	0.3346859360094447
0.2485232874614568	0.5000857509501908	0.3292763757024605
0.7579229819712614	0.5000908825960459	0.3292167571906057
0.7510732608673798	0.8381303538466297	0.3949987094916066
0.2480966934209902	0.1623209684060525	0.3950378157325381
0.2480407844466741	0.8380581757714658	0.3949948358793384
0.7509622045473462	0.1622416422965579	0.3950359549108992
0.7477270142167147	0.5001424553569920	0.3940660504919100
0.2529516312011711	0.5001437719573292	0.3941420550180978
0.4996718854900972	0.0000551808443969	0.4211984647454454
0.5002448176595216	0.3324279102643135	0.4191688438962435
0.0000290131250544	0.3327095772044000	0.4212851346651256
0.0000274363276940	0.6676253518051729	0.4213316351853768
0.9997335448451782	0.0001303410827764	0.4211399444892900
0.5002444622397177	0.6681400859170110	0.4189689177263556
0.2527968016466761	0.3333921619772525	0.4728911351759265

0.7469748914139475	0.3334206889266117	0.4729246914671243
0.2484667698852607	-0.0000445532336292	0.4733707704743312
0.7465997764563957	0.6664871680402593	0.4729311738971093
0.7512190015665222	-0.0000369304833815	0.4733764941957179
0.2531856066860717	0.6665021428893843	0.4728955575654641
0.4998228919107773	0.4995567077706128	0.5028027681999285
0.4998680718045554	0.1638848839186697	0.4963017474722261
-0.0001345453552485	0.5002979152527899	0.4956841485653242
0.4998665967407543	0.8360662517370699	0.4963918701434604
-0.0001531904008751	0.1688601099680655	0.4966867696794623
-0.0001393210658245	0.8314262499024553	0.4966806740914348
0.4994457803177523	0.4939714973701236	0.5657456741027143
0.4992783348112166	0.3789059453721725	0.5857732066336087
0.4993608075154594	0.6072310064704286	0.5864902380570998

The structural information of *CH₃

8.2384996414000007	0.0000000000000000	0.0000000000000000			
0.0000000000000000	8.0431003571000002	0.0000000000000000			
0.0000000000000000	0.0000000000000000	29.7859992980999984			
Ta	Na	O	Ru	C	H
12	12	36	24	1	3

Direct

0.2509500000000031	0.5000000000000000	0.0000000000000000
0.2509500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.5000000000000000	0.0000000000000000
0.7505700000000033	0.0000000000000000	0.1331699999999998
0.2505700000000033	0.5000000000000000	0.1331699999999998
0.2505700000000033	0.0000000000000000	0.1331699999999998
0.7505700000000033	0.5000000000000000	0.1331699999999998
0.7387291272647766	0.0000243967078935	0.2673668630468226
0.2393082963262475	0.5000108585119366	0.2655437614255474
0.7402850971777701	0.5000223527992779	0.2655857093354084
0.2390626454092259	0.0000291231893201	0.2674121815651516
0.0007599999999996	0.7500000000000000	0.0665800000000019
0.0007599999999996	0.2500000000000000	0.0665800000000019

0.5007599999999996	0.2500000000000000	0.0665800000000019
0.5007599999999996	0.7500000000000000	0.0665800000000019
0.5003799999999998	0.2500000000000000	0.1997500000000016
0.0003799999999998	0.7500000000000000	0.1997500000000016
0.0003799999999998	0.2500000000000000	0.1997500000000016
0.5003799999999998	0.7500000000000000	0.1997500000000016
0.4912168611054757	0.2539382367033740	0.3171441751437739
0.9911624968678662	0.7413409346357710	0.3178882736504358
0.4912197500479017	0.7460378766437187	0.3171593184731240
0.9911678284238634	0.2586443684708132	0.3178772567070123
0.2509500000000031	0.7500000000000000	0.0000000000000000
0.2509500000000031	0.2500000000000000	0.0000000000000000
0.7509500000000031	0.7500000000000000	0.0000000000000000
0.0009500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.2500000000000000	0.0000000000000000
0.0009500000000031	0.5000000000000000	0.0000000000000000
0.5009500000000031	0.5000000000000000	0.0000000000000000
0.5009500000000031	0.0000000000000000	0.0000000000000000
0.7507599999999996	0.0000000000000000	0.0665800000000019
0.7507599999999996	0.5000000000000000	0.0665800000000019
0.2507599999999996	0.5000000000000000	0.0665800000000019
0.2507599999999996	0.0000000000000000	0.0665800000000019
0.0005700000000033	0.0000000000000000	0.1331699999999998
0.5005700000000033	0.0000000000000000	0.1331699999999998
0.7505700000000033	0.2500000000000000	0.1331699999999998
0.2505700000000033	0.7500000000000000	0.1331699999999998
0.5005700000000033	0.5000000000000000	0.1331699999999998
0.2505700000000033	0.2500000000000000	0.1331699999999998
0.7505700000000033	0.7500000000000000	0.1331699999999998
0.0005700000000033	0.5000000000000000	0.1331699999999998
0.2503799999999998	0.5000000000000000	0.1997500000000016
0.7503799999999998	0.5000000000000000	0.1997500000000016
0.2503799999999998	0.0000000000000000	0.1997500000000016
0.7503799999999998	0.0000000000000000	0.1997500000000016
0.7507017570699456	0.2478177891968431	0.2661773850119377

0.0010962968842404	0.5000393714783248	0.2633277207569255
0.0017463280708559	0.0000394707746810	0.2674595617713835
0.2514037710701525	0.2478180718795855	0.2661834186039901
0.7506813860705210	0.7522734053967107	0.2661857699077145
0.2514128668268422	0.7522510339215028	0.2661940186700167
0.5016295476540593	0.0000547691252958	0.2663914163054646
0.5014422110335280	0.5000298640262709	0.2652508930148178
0.7463163001598931	0.0001771546158876	0.3348052559509077
0.2550446166255345	0.0001482382551732	0.3347730220614646
0.2452336828516622	0.5000591890234395	0.3291953318096552
0.7595622309133148	0.5001186838470451	0.3290846315420042
0.7498523436130243	0.8385281812224247	0.3946461767848403
0.2463045941734615	0.1623009046225883	0.3946881974486145
0.2463450959447975	0.8384687118566279	0.3946576120783415
0.7498915495980630	0.1622327025826405	0.3946682374411825
0.7463893975708344	0.5003772769277823	0.3939494209007182
0.2513990901222805	0.5003606878887710	0.3940761492086782
0.4982663852799593	0.0004118109600853	0.4210835768070216
0.4988502635035282	0.3315116236742085	0.4182143513545057
-0.0015734731676209	0.3328730871316676	0.4214134408127177
-0.0015431124423259	0.6679358622242505	0.4214025825314844
0.9981080510735030	0.0003849443582166	0.4211124509557084
0.4988501550229109	0.6692089045379839	0.4182606612802764
0.2538809135109287	0.3352157626217813	0.4728265195998750
0.7425809467285978	0.3352167645336270	0.4729279208679016
0.2469517109672983	0.0004436305438982	0.4731525415528709
0.7426970870876358	0.6656170078842021	0.4729205196153311
0.7494683405247049	0.0003402396032603	0.4732654249219108
0.2537891994532128	0.6656484764658362	0.4728300124142641
0.4979483044333834	0.5004509602447115	0.5024585742008909
0.4982308637425578	0.1641602990620482	0.4967366975380146
-0.0019265468824883	0.5003545614939884	0.4958783180959725
0.4982252657992238	0.8366070787286212	0.4967055478397068
-0.0017532039631052	0.1703689286374993	0.4964050591871728
-0.0017363584441633	0.8304049163822781	0.4964108386233544

0.4932385640581942	0.5021277948455241	0.5725782499207444
0.5511827850680009	0.3892599317299606	0.5858901971288626
0.5564393161663029	0.6126136083933659	0.5855271244497534
0.3647103697794253	0.5055263863883704	0.5825629639005673

The structural information of *CH₄

8.2384996414000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0431003571000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.7859992980999984

Ta	Na	O	Ru	C	H
12	12	36	24	1	4

Direct

0.2509500000000031	0.5000000000000000	0.0000000000000000
0.2509500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.5000000000000000	0.0000000000000000
0.7505700000000033	0.0000000000000000	0.1331699999999998
0.2505700000000033	0.5000000000000000	0.1331699999999998
0.2505700000000033	0.0000000000000000	0.1331699999999998
0.7505700000000033	0.5000000000000000	0.1331699999999998
0.7390756182990236	-0.0000238532100054	0.2673671544735950
0.2401978368453767	0.4999803202410644	0.2655983363140787
0.7400317543064213	0.4999477040807302	0.2655902222218299
0.2393902171069589	-0.0000143777203841	0.2673922097087894
0.0007599999999996	0.7500000000000000	0.0665800000000019
0.0007599999999996	0.2500000000000000	0.0665800000000019
0.5007599999999996	0.2500000000000000	0.0665800000000019
0.5007599999999996	0.7500000000000000	0.0665800000000019
0.5003799999999998	0.2500000000000000	0.1997500000000016
0.0003799999999998	0.7500000000000000	0.1997500000000016
0.0003799999999998	0.2500000000000000	0.1997500000000016
0.5003799999999998	0.7500000000000000	0.1997500000000016
0.4915258721903522	0.2560172621245205	0.3176792478458873
0.9915398860644770	0.7434482598529565	0.3175709233000648
0.4914121146432729	0.7439203245950025	0.3176910436373197
0.9914910528640843	0.2564552445676322	0.3175642424362488

0.2509500000000031	0.7500000000000000	0.0000000000000000
0.2509500000000031	0.2500000000000000	0.0000000000000000
0.7509500000000031	0.7500000000000000	0.0000000000000000
0.0009500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.2500000000000000	0.0000000000000000
0.0009500000000031	0.5000000000000000	0.0000000000000000
0.5009500000000031	0.5000000000000000	0.0000000000000000
0.5009500000000031	0.0000000000000000	0.0000000000000000
0.7507599999999996	0.0000000000000000	0.0665800000000019
0.7507599999999996	0.5000000000000000	0.0665800000000019
0.2507599999999996	0.5000000000000000	0.0665800000000019
0.2507599999999996	0.0000000000000000	0.0665800000000019
0.0005700000000033	0.0000000000000000	0.1331699999999998
0.5005700000000033	0.0000000000000000	0.1331699999999998
0.7505700000000033	0.2500000000000000	0.1331699999999998
0.2505700000000033	0.7500000000000000	0.1331699999999998
0.5005700000000033	0.5000000000000000	0.1331699999999998
0.2505700000000033	0.2500000000000000	0.1331699999999998
0.7505700000000033	0.7500000000000000	0.1331699999999998
0.0005700000000033	0.5000000000000000	0.1331699999999998
0.2503799999999998	0.5000000000000000	0.1997500000000016
0.7503799999999998	0.5000000000000000	0.1997500000000016
0.2503799999999998	0.0000000000000000	0.1997500000000016
0.7503799999999998	0.0000000000000000	0.1997500000000016
0.7515826079346165	0.2477374083927331	0.2662115561430768
0.0015766932503627	0.5000169285794119	0.2644142674218750
0.0019596650592244	-0.0000482533195372	0.2672031004179453
0.2512978923556333	0.2478567650644981	0.2662080837283330
0.7515258439074295	0.7521406459955132	0.2662082442263665
0.2513644179767386	0.7522768052433193	0.2662064966947427
0.5018567620229747	0.0000164381682239	0.2666622243090208
0.5015294295893390	0.4999509314214425	0.2642965307579380
0.7486517576279853	-0.0002602820598730	0.3347365664671262
0.2528621520671051	0.0002937025784216	0.3347231643185343
0.2532085464366894	0.5002411882086507	0.3292072013288731

0.7522830824455059	0.4997857217096950	0.3292220479989807
0.7489009821920286	0.8383934106032910	0.3943885813558672
0.2480980560226875	0.1617954272632756	0.3943922120841726
0.2480476709022686	0.8382440823389735	0.3944761620233665
0.7488888443657172	0.1619644625329364	0.3944883284519982
0.7482629574275841	0.5000976553062754	0.3941624591856074
0.2501318901872649	0.5000360138790071	0.3941667635887426
0.4986765936953997	0.0000757345145162	0.4208534183396901
0.4988701325534480	0.3320070704243010	0.4205200798282610
-0.0008640039587942	0.3316276528714812	0.4205038266308743
-0.0012816475497743	0.6685532940354589	0.4205023689077111
-0.0014235984311326	0.0001258230761150	0.4204165884759426
0.4993734258433847	0.6681585112263211	0.4205156312316239
0.2486710415851975	0.3326188186853145	0.4726223856406509
0.7488704809158107	0.3329175070355233	0.4725513269818875
0.2475662738744281	0.0000122810049715	0.4731435613918901
0.7488889758137769	0.6674943523685115	0.4727279782767698
0.7500295796599603	0.0001253713904694	0.4731895411469159
0.2486960812113976	0.6673351997659983	0.4724375463527367
0.4985806381848290	0.5000681032013747	0.4979264257464561
0.4987825016357588	0.1650634086796967	0.4961675600110542
-0.0012722688980645	0.5000919263462056	0.4965013608739734
0.4988333276122248	0.8350896563227163	0.4961671448960693
-0.0013354263040848	0.1681333308276702	0.4966382938088272
-0.0010888646900215	0.8320728133869676	0.4966361428003509
0.4932152162007718	0.4999303168159580	0.5862374433248226
0.3835788721760678	0.5231806731078541	0.5652329348911200
0.6060071915945981	0.4768182018711786	0.5665774163462528
0.5135488505382215	0.6106566256687170	0.6068907015461684
0.4692607985842002	0.3891609583043003	0.6065717977367636

The structural information of Rh@NaTaO₃

7.7705998421000002	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.7708997726000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.8873004912999995

Ta	Na	O	Rh
12	12	36	16

Direct

0.2505700000000033	0.7500000000000000	0.0000000000000000
0.2505700000000033	0.2500000000000000	0.0000000000000000
0.7505700000000033	0.2500000000000000	0.0000000000000000
0.7505700000000033	0.7500000000000000	0.0000000000000000
0.7501900000000035	0.2500000000000000	0.1373099999999994
0.2501900000000035	0.7500000000000000	0.1373099999999994
0.2501900000000035	0.2500000000000000	0.1373099999999994
0.7501900000000035	0.7500000000000000	0.1373099999999994
0.7499680691023030	0.2499384902885561	0.2772793045010701
0.2499688249913102	0.7499455081518990	0.2772724007155032
0.7499657384683842	0.7499427805560048	0.2772713462168671
0.2499733105127238	0.2499420010757832	0.2772804406274154
0.0003799999999998	0.5000000000000000	0.0686600000000013
0.0003799999999998	0.0000000000000000	0.0686600000000013
0.5003799999999998	0.0000000000000000	0.0686600000000013
0.5003799999999998	0.5000000000000000	0.0686600000000013
0.5000000000000000	0.0000000000000000	0.2059700000000007
0.0000000000000000	0.5000000000000000	0.2059700000000007
0.0000000000000000	0.0000000000000000	0.2059700000000007
0.5000000000000000	0.5000000000000000	0.2059700000000007
0.9992551613638071	-0.0009585432948471	0.3295057801766892
0.4992517945164918	0.4990080031238234	0.3294970258224106
0.9992497943435539	0.4990083314783619	0.3294949781597798
0.4992593115191272	-0.0009601363359842	0.3295076507950425
0.2505700000000033	0.5000000000000000	0.0000000000000000
0.5005700000000033	0.7500000000000000	0.0000000000000000
0.0005700000000033	0.2500000000000000	0.0000000000000000
0.2505700000000033	0.0000000000000000	0.0000000000000000

0.5005700000000033	0.2500000000000000	0.0000000000000000
0.0005700000000033	0.7500000000000000	0.0000000000000000
0.7505700000000033	0.5000000000000000	0.0000000000000000
0.7505700000000033	0.0000000000000000	0.0000000000000000
0.7503799999999998	0.2500000000000000	0.0686600000000013
0.7503799999999998	0.7500000000000000	0.0686600000000013
0.2503799999999998	0.2500000000000000	0.0686600000000013
0.2503799999999998	0.7500000000000000	0.0686600000000013
0.5001900000000035	0.2500000000000000	0.1373099999999994
0.0001900000000035	0.2500000000000000	0.1373099999999994
0.7501900000000035	0.0000000000000000	0.1373099999999994
0.2501900000000035	0.5000000000000000	0.1373099999999994
0.5001900000000035	0.7500000000000000	0.1373099999999994
0.7501900000000035	0.5000000000000000	0.1373099999999994
0.2501900000000035	0.0000000000000000	0.1373099999999994
0.0001900000000035	0.7500000000000000	0.1373099999999994
0.2500000000000000	0.7500000000000000	0.2059700000000007
0.2500000000000000	0.2500000000000000	0.2059700000000007
0.7500000000000000	0.2500000000000000	0.2059700000000007
0.7500000000000000	0.7500000000000000	0.2059700000000007
0.5000311089845745	0.7500159300944790	0.2742049350311989
0.0000304838651715	0.2500192658858589	0.2741998264836532
0.7499089813894241	0.0000602177036606	0.2742028962321130
0.2499032051087645	0.5000798054877490	0.2742034786198058
0.7499062799382792	0.5000748279510115	0.2742037190936802
0.5000369188310787	0.2500156326423812	0.2742002250228052
0.0000342690954861	0.7500131423649838	0.2742056691727115
0.2499004288987915	0.0000565270777422	0.2742031419620345
0.7507404197726408	0.2508900239880215	0.3440288918622580
0.2507305853113454	0.2508823305638129	0.3440291895945196
0.2507336513516467	0.7508799012729669	0.3440349212071965
0.7507412812909561	0.7508883465397773	0.3440350271466370
0.5020309657592894	0.0026906138275334	0.4239147868965456
0.2518178141073347	0.2523758355133593	0.4148440692225169
0.5020321445051313	0.5026916519239746	0.4239199582837161

0.0020313381964374	0.0026973861582607	0.4239156301204908
0.7518176411057131	0.2523760086564499	0.4148439732008865
0.2518133714416892	0.7523580482974616	0.4148418208449287
0.7518096169479301	0.7523672873477231	0.4148413341396115
0.0020355149002903	0.5026844574933595	0.4239208857102538
0.5018801467708063	0.2526539713849866	0.4793088152272462
0.2520414124077173	0.5024710146734328	0.4793058491422887
0.7520069934009007	0.0024830190008338	0.4793191831220865
0.2520371212095055	0.0024794734296741	0.4793193651973858
0.5018878813073009	0.7527096111765528	0.4793072349524600
0.0018819907864275	0.2526516000288093	0.4793060974999818
0.7520095926486902	0.5024656831509324	0.4793033358829851
0.0018796692541292	0.7527127035306739	0.4793010208072558

The structural information of *CO₂

7.7705998421000002	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.7708997726000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.8873004912999995

Ta	Na	O	Rh	C
12	12	38	16	1

Direct

0.2505700000000033	0.7500000000000000	0.0000000000000000
0.2505700000000033	0.2500000000000000	0.0000000000000000
0.7505700000000033	0.2500000000000000	0.0000000000000000
0.7505700000000033	0.7500000000000000	0.0000000000000000
0.7501900000000035	0.2500000000000000	0.1373099999999994
0.2501900000000035	0.7500000000000000	0.1373099999999994
0.2501900000000035	0.2500000000000000	0.1373099999999994
0.7501900000000035	0.7500000000000000	0.1373099999999994
0.7511995152990089	0.2529613570092713	0.2766614794729290
0.2511555374081930	0.7531677057746151	0.2764872069255299
0.7530551912118719	0.7512770079193561	0.2766930595249351
0.2535943003245821	0.2517509495121829	0.2765339136952047
0.0003799999999998	0.5000000000000000	0.0686600000000013
0.0003799999999998	0.0000000000000000	0.0686600000000013
0.5003799999999998	0.0000000000000000	0.0686600000000013

0.5003799999999998	0.5000000000000000	0.0686600000000013
0.5000000000000000	0.0000000000000000	0.2059700000000007
0.0000000000000000	0.5000000000000000	0.2059700000000007
0.0000000000000000	0.0000000000000000	0.2059700000000007
0.5000000000000000	0.5000000000000000	0.2059700000000007
0.0029795865160261	0.0173252114704227	0.3317115892754641
0.5025019534348421	0.5158056928232390	0.3322098219950429
0.0153191772328051	0.5051095438999973	0.3320087769699626
0.5138101647568390	0.0042889540799772	0.3320714651718157
0.2505700000000033	0.5000000000000000	0.0000000000000000
0.5005700000000033	0.7500000000000000	0.0000000000000000
0.0005700000000033	0.2500000000000000	0.0000000000000000
0.2505700000000033	0.0000000000000000	0.0000000000000000
0.5005700000000033	0.2500000000000000	0.0000000000000000
0.0005700000000033	0.7500000000000000	0.0000000000000000
0.7505700000000033	0.5000000000000000	0.0000000000000000
0.7505700000000033	0.0000000000000000	0.0000000000000000
0.7503799999999998	0.2500000000000000	0.0686600000000013
0.7503799999999998	0.7500000000000000	0.0686600000000013
0.2503799999999998	0.2500000000000000	0.0686600000000013
0.2503799999999998	0.7500000000000000	0.0686600000000013
0.5001900000000035	0.2500000000000000	0.1373099999999994
0.0001900000000035	0.2500000000000000	0.1373099999999994
0.7501900000000035	0.0000000000000000	0.1373099999999994
0.2501900000000035	0.5000000000000000	0.1373099999999994
0.5001900000000035	0.7500000000000000	0.1373099999999994
0.7501900000000035	0.5000000000000000	0.1373099999999994
0.2501900000000035	0.0000000000000000	0.1373099999999994
0.0001900000000035	0.7500000000000000	0.1373099999999994
0.2500000000000000	0.7500000000000000	0.2059700000000007
0.2500000000000000	0.2500000000000000	0.2059700000000007
0.7500000000000000	0.2500000000000000	0.2059700000000007
0.7500000000000000	0.7500000000000000	0.2059700000000007
0.5004072393557943	0.8010534310649132	0.2739020704525822
0.0006293346788660	0.3007407205934061	0.2740894736267912

0.8013697505208097	0.9998670496634227	0.2737036630192419
0.3016714602928487	0.5002724430621781	0.2734960391205403
0.6985875786265525	0.4999891537024190	0.2733493579319345
0.5007679611071336	0.1979706245455309	0.2730197734915212
0.0004698434773824	0.6982947295820029	0.2730351167243973
0.1989569376208976	0.0003151105265286	0.2733397581401139
0.7477529679390059	0.2433591737506302	0.3435612073611167
0.2485449761572529	0.2476109332869853	0.3434221447755897
0.2469907724338778	0.7433022762168100	0.3433912425333498
0.7461877789611842	0.7454782448761893	0.3435824737268625
0.6744431874957715	0.4155814381379534	0.5525579684614829
0.4941333434706925	0.2019631058822733	0.5782787283816996
0.4807696595480378	0.9857204751443109	0.4246611850836660
0.2378747395555658	0.2289913981045464	0.4140323467818812
0.4936269437333228	0.4795874780300676	0.4249474947467000
0.9927328679704364	0.9780000159694593	0.4240167356976020
0.7333323050107965	0.2341223057356466	0.4143993725732359
0.2379688011600317	0.7357454508078705	0.4141274946276368
0.7393800190345740	0.7305467154672328	0.4146237033830245
0.9763651389901117	0.4861636928503991	0.4244111248314661
0.4906991615050156	0.2379758313883495	0.4828425981738343
0.2351498069877082	0.4835312075818549	0.4766828260903171
0.7388872982220769	0.9830734011810149	0.4775259694823416
0.2344601523248631	0.9848947311971823	0.4816975679854292
0.4894472059484970	0.7344455279777710	0.4781114374941697
0.9884053807355657	0.2317717715912067	0.4776193599941254
0.7402393608700382	0.4873388839329031	0.4853484815152018
0.9885112846645813	0.7336275531778740	0.4806396923179320
0.5646925806662512	0.2918577705796664	0.5492049011618778

The structural information of *COOH

7.7705998421000002	0.0000000000000000	0.0000000000000000			
0.0000000000000000	7.7708997726000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	28.8873004912999995			
Ta	Na	O	Rh	C	H
12	12	38	16	1	1

Direct

0.2505700000000033	0.7500000000000000	0.0000000000000000
0.2505700000000033	0.2500000000000000	0.0000000000000000
0.7505700000000033	0.2500000000000000	0.0000000000000000
0.7505700000000033	0.7500000000000000	0.0000000000000000
0.7501900000000035	0.2500000000000000	0.1373099999999994
0.2501900000000035	0.7500000000000000	0.1373099999999994
0.2501900000000035	0.2500000000000000	0.1373099999999994
0.7501900000000035	0.7500000000000000	0.1373099999999994
0.7521516282471414	0.2519581407867094	0.2763930478097275
0.2513247057472812	0.7512920964242850	0.2767537083355852
0.7524750345838265	0.7498675198342937	0.2767249218020862
0.2518907199613320	0.2501431016320617	0.2764958277387087
0.0003799999999998	0.5000000000000000	0.0686600000000013
0.0003799999999998	0.0000000000000000	0.0686600000000013
0.5003799999999998	0.0000000000000000	0.0686600000000013
0.5003799999999998	0.5000000000000000	0.0686600000000013
0.5000000000000000	0.0000000000000000	0.2059700000000007
0.0000000000000000	0.5000000000000000	0.2059700000000007
0.0000000000000000	0.0000000000000000	0.2059700000000007
0.5000000000000000	0.5000000000000000	0.2059700000000007
0.0035426259414359	0.0061077577277522	0.3318844134623946
0.5033225869548814	0.5053573504096287	0.3307506441448262
0.0127943736126681	0.4987552451998694	0.3329207515490201
0.5141556021156869	0.0000739621064862	0.3318539361610933
0.2505700000000033	0.5000000000000000	0.0000000000000000
0.5005700000000033	0.7500000000000000	0.0000000000000000
0.0005700000000033	0.2500000000000000	0.0000000000000000
0.2505700000000033	0.0000000000000000	0.0000000000000000
0.5005700000000033	0.2500000000000000	0.0000000000000000
0.0005700000000033	0.7500000000000000	0.0000000000000000
0.7505700000000033	0.5000000000000000	0.0000000000000000
0.7505700000000033	0.0000000000000000	0.0000000000000000
0.7503799999999998	0.2500000000000000	0.0686600000000013
0.7503799999999998	0.7500000000000000	0.0686600000000013

0.2503799999999998	0.2500000000000000	0.0686600000000013
0.2503799999999998	0.7500000000000000	0.0686600000000013
0.50019000000000035	0.2500000000000000	0.1373099999999994
0.00019000000000035	0.2500000000000000	0.1373099999999994
0.75019000000000035	0.0000000000000000	0.1373099999999994
0.25019000000000035	0.5000000000000000	0.1373099999999994
0.50019000000000035	0.7500000000000000	0.1373099999999994
0.75019000000000035	0.5000000000000000	0.1373099999999994
0.25019000000000035	0.0000000000000000	0.1373099999999994
0.00019000000000035	0.7500000000000000	0.1373099999999994
0.25000000000000000	0.7500000000000000	0.2059700000000007
0.25000000000000000	0.2500000000000000	0.2059700000000007
0.75000000000000000	0.2500000000000000	0.2059700000000007
0.75000000000000000	0.7500000000000000	0.2059700000000007
0.5001678424989291	0.8006084989224054	0.2737610212685251
0.0002895411341841	0.3019057976528413	0.2730822120157384
0.8007315079080397	0.0002750435477650	0.2738270310685236
0.3009229141368847	0.5002134079374881	0.2735066126554399
0.6986140593687574	0.5004015123618311	0.2728161025925677
0.5002692473039378	0.1994582815079302	0.2738789154966669
0.0002170841402998	0.6982959697101252	0.2736826766850952
0.1988915219467461	0.0001611221449171	0.2732694245937219
0.7503740674553611	0.2508434186049884	0.3432918041272419
0.2426667730941993	0.2511698115582185	0.3434034294320828
0.2467103912427099	0.7477812835944088	0.3436921738014012
0.7461201950658516	0.7494752003954288	0.3436616448493417
0.9418240014088691	0.6483339847113329	0.5529421399294822
0.7717270027798224	0.4489244002665413	0.5833860441281015
0.4816949409760710	0.0011402248627842	0.4243902436871040
0.2381323171545438	0.2455235486315595	0.4143496409248389
0.4901488976687455	0.4939521768884693	0.4226970820933946
0.9921175200483221	0.9889436530152244	0.4247309365672364
0.7338976378184290	0.2474997316888876	0.4137839735495535
0.2341469875060386	0.7521574504649039	0.4147530595369062
0.7396959073000583	0.7450097655232520	0.4147367736288399

0.9830809163907208	0.5082766718217728	0.4262805727522663
0.4904438405206671	0.2494674315669776	0.4803953979845234
0.2425571793565792	0.4985883126137088	0.4771623139596027
0.7360836768939119	-0.0015439160191188	0.4777003409946575
0.2385512834312946	0.0014613594827134	0.4813816653146876
0.4893264516904007	0.7465378103553764	0.4777446235151330
0.9842588174016405	0.2470032016700562	0.4767100971646114
0.7328208063362706	0.4927260748997846	0.4838667936096751
0.9925823826934673	0.7575283924875427	0.4859957048455664
0.8286129660243129	0.5349128453536135	0.5457464599288290
0.6880163885463194	0.3643798756698476	0.5717260732899831

The structural information of *CO

7.7705998421000002	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.7708997726000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.8873004912999995

Ta	Na	O	Rh	C
12	12	37	16	1

Direct

0.2505700000000033	0.7500000000000000	0.0000000000000000
0.2505700000000033	0.2500000000000000	0.0000000000000000
0.7505700000000033	0.2500000000000000	0.0000000000000000
0.7505700000000033	0.7500000000000000	0.0000000000000000
0.7501900000000035	0.2500000000000000	0.1373099999999994
0.2501900000000035	0.7500000000000000	0.1373099999999994
0.2501900000000035	0.2500000000000000	0.1373099999999994
0.7501900000000035	0.7500000000000000	0.1373099999999994
0.7509798533340877	0.2495568233758262	0.2766591095754819
0.2511837088382536	0.7490970039315239	0.2766531085251581
0.7502880915822217	0.7484969126248670	0.2766423969874006
0.2505824432735618	0.2490590856958067	0.2766626656613358
0.0003799999999998	0.5000000000000000	0.0686600000000013
0.0003799999999998	0.0000000000000000	0.0686600000000013
0.5003799999999998	0.0000000000000000	0.0686600000000013
0.5003799999999998	0.5000000000000000	0.0686600000000013
0.5000000000000000	0.0000000000000000	0.2059700000000007

0.0000000000000000	0.5000000000000000	0.2059700000000007
0.0000000000000000	0.0000000000000000	0.2059700000000007
0.5000000000000000	0.5000000000000000	0.2059700000000007
0.9995165748918202	0.9944167807511602	0.3318510786642120
0.4988485308990121	0.4951725772193742	0.3320118047602443
0.0071718980927835	0.4976372276718924	0.3318167586239084
0.5039952569421933	0.9976953214087465	0.3318419858051385
0.2505700000000033	0.5000000000000000	0.0000000000000000
0.5005700000000033	0.7500000000000000	0.0000000000000000
0.0005700000000033	0.2500000000000000	0.0000000000000000
0.2505700000000033	0.0000000000000000	0.0000000000000000
0.5005700000000033	0.2500000000000000	0.0000000000000000
0.0005700000000033	0.7500000000000000	0.0000000000000000
0.7505700000000033	0.5000000000000000	0.0000000000000000
0.7505700000000033	0.0000000000000000	0.0000000000000000
0.7503799999999998	0.2500000000000000	0.0686600000000013
0.7503799999999998	0.7500000000000000	0.0686600000000013
0.2503799999999998	0.2500000000000000	0.0686600000000013
0.2503799999999998	0.7500000000000000	0.0686600000000013
0.5001900000000035	0.2500000000000000	0.1373099999999994
0.0001900000000035	0.2500000000000000	0.1373099999999994
0.7501900000000035	0.0000000000000000	0.1373099999999994
0.2501900000000035	0.5000000000000000	0.1373099999999994
0.5001900000000035	0.7500000000000000	0.1373099999999994
0.7501900000000035	0.5000000000000000	0.1373099999999994
0.2501900000000035	0.0000000000000000	0.1373099999999994
0.0001900000000035	0.7500000000000000	0.1373099999999994
0.2500000000000000	0.7500000000000000	0.2059700000000007
0.2500000000000000	0.2500000000000000	0.2059700000000007
0.7500000000000000	0.2500000000000000	0.2059700000000007
0.7500000000000000	0.7500000000000000	0.2059700000000007
0.5002528315826283	0.8010617550180394	0.2733156139007397
0.0001981952011420	0.3006979838545244	0.2732567517211448
0.8005838630113097	0.9997479013979456	0.2736616427421289
0.3012339174171476	0.4997918330293162	0.2730881056528728

0.6982387918766388	0.4997302700741328	0.2733447248562030
0.5002684063060856	0.1985926639377675	0.2737322086795917
0.0001701283530150	0.6989706033548635	0.2736821478621539
0.1992917853289877	0.9997783412734836	0.2739211586193770
0.7502865320989103	0.2523095323675176	0.3435891570952250
0.2497626765496886	0.2556417528315621	0.3435312672437285
0.2504823933719084	0.7476601277654833	0.3435549418473835
0.7494344912399450	0.7508033952683991	0.3435774921425613
0.7264823944277130	0.5004226287293287	0.5916923952748553
0.4931125268090776	0.0059460024439281	0.4247481360921447
0.2498723176291233	0.2509074229009829	0.4148137066648965
0.5066325093949333	0.5059950645973555	0.4249892976926374
0.0061419230365348	0.0059377468557984	0.4246827520783343
0.7497885579787568	0.2552984509759117	0.4145192041579793
0.2499189473718890	0.7596922189491777	0.4147883759894314
0.7497204784305128	0.7550213036434295	0.4145519869663051
0.9915856449087135	0.5060159498529434	0.4244799734595917
0.5024400402443778	0.2546987488963022	0.4795023299966591
0.2486873788772089	0.5054034107409685	0.4768332961217631
0.7498055633274959	0.0055176921110844	0.4777457511787440
0.2495080083254713	0.0054368303857312	0.4818977648135123
0.5023732133354627	0.7571970808613350	0.4795260193223971
0.9974913766225009	0.2553086304835805	0.4794303634641551
0.7518673063785238	0.5056111977289089	0.4880930060039264
0.9975317417196071	0.7566044303697241	0.4794595023503002
0.7338267520046673	0.5025371654311067	0.5512672171002402

The structural information of *COH

7.7705998421000002	0.0000000000000000	0.0000000000000000			
0.0000000000000000	7.7708997726000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	28.8873004912999995			
Ta	Na	O	Rh	C	H
12	12	37	16	1	1
Direct					
0.2505700000000033	0.7500000000000000	0.0000000000000000			
0.2505700000000033	0.2500000000000000	0.0000000000000000			

0.75057000000000033	0.25000000000000000	0.00000000000000000
0.75057000000000033	0.75000000000000000	0.00000000000000000
0.75019000000000035	0.25000000000000000	0.13730999999999994
0.25019000000000035	0.75000000000000000	0.13730999999999994
0.25019000000000035	0.25000000000000000	0.13730999999999994
0.75019000000000035	0.75000000000000000	0.13730999999999994
0.7523286993269083	0.2469341017711681	0.2765972685994348
0.2524049447942783	0.7472875250154956	0.2765911939625263
0.7495980265866520	0.7461946893352512	0.2765433918127442
0.2503231270205430	0.2466334120950449	0.2765549323967649
0.00037999999999998	0.50000000000000000	0.06866000000000013
0.00037999999999998	0.00000000000000000	0.06866000000000013
0.50037999999999998	0.00000000000000000	0.06866000000000013
0.50037999999999998	0.50000000000000000	0.06866000000000013
0.50000000000000000	0.00000000000000000	0.20597000000000007
0.00000000000000000	0.50000000000000000	0.20597000000000007
0.00000000000000000	0.00000000000000000	0.20597000000000007
0.50000000000000000	0.50000000000000000	0.20597000000000007
0.0013874739270241	0.9808801980393533	0.3317218120507711
0.5012225115305414	0.4823818058091998	0.3322038991211645
0.0065289313299719	0.4901870251202319	0.3316792417163768
0.5052556085164086	0.9897890402592352	0.3318556924980979
0.25057000000000033	0.50000000000000000	0.00000000000000000
0.50057000000000033	0.75000000000000000	0.00000000000000000
0.00057000000000033	0.25000000000000000	0.00000000000000000
0.25057000000000033	0.00000000000000000	0.00000000000000000
0.50057000000000033	0.25000000000000000	0.00000000000000000
0.00057000000000033	0.75000000000000000	0.00000000000000000
0.75057000000000033	0.50000000000000000	0.00000000000000000
0.75057000000000033	0.00000000000000000	0.00000000000000000
0.75037999999999998	0.25000000000000000	0.06866000000000013
0.75037999999999998	0.75000000000000000	0.06866000000000013
0.25037999999999998	0.25000000000000000	0.06866000000000013
0.25037999999999998	0.75000000000000000	0.06866000000000013
0.50019000000000035	0.25000000000000000	0.13730999999999994

0.00019000000000035	0.2500000000000000	0.1373099999999994
0.75019000000000035	0.0000000000000000	0.1373099999999994
0.25019000000000035	0.5000000000000000	0.1373099999999994
0.50019000000000035	0.7500000000000000	0.1373099999999994
0.75019000000000035	0.5000000000000000	0.1373099999999994
0.25019000000000035	0.0000000000000000	0.1373099999999994
0.00019000000000035	0.7500000000000000	0.1373099999999994
0.25000000000000000	0.7500000000000000	0.2059700000000007
0.25000000000000000	0.2500000000000000	0.2059700000000007
0.75000000000000000	0.2500000000000000	0.2059700000000007
0.75000000000000000	0.7500000000000000	0.2059700000000007
0.5003397610008878	0.8008738934891882	0.2724022921878297
0.0006081840215053	0.3003629374460528	0.2726158832894063
0.8014335206119644	0.9991366448497080	0.2736307752382339
0.3015644036414005	0.4996081794985056	0.2735139165982663
0.6987659464216559	0.4990742181045383	0.2733238081216531
0.5005814915860824	0.1979668308700761	0.2742752732316400
0.0003401748257969	0.6987164986081362	0.2745543516975382
0.1991035156160720	0.9995101326239889	0.2734596639292477
0.7520153571763715	0.2559295503587253	0.3435053979154931
0.2487472171080193	0.2582553049773468	0.3434238084237076
0.2525300755289268	0.7565555816991536	0.3435538248673072
0.7448925087443039	0.7556184873258917	0.3434253594133470
0.6599169132928704	0.3657391383009320	0.5746524920436590
0.4896546602078941	0.0317581845531591	0.4239248569815343
0.2408465645388411	0.2706191385515166	0.4143073309089720
0.4949187967838456	0.5241659625514427	0.4246932210877038
0.9978039481113442	0.0221184149825072	0.4239835494084800
0.7413266950268970	0.2759619076694040	0.4140020320065426
0.2443836928846581	0.7744555325456045	0.4144471801492038
0.7482560234893055	0.7765428751265041	0.4141603562760443
0.9909159493842512	0.5313384489114638	0.4236046334598279
0.4947775370519270	0.2756452700771249	0.4844922818073766
0.2410536230671547	0.5221185990498113	0.4778501927400473
0.7446275005336873	0.0238698636534672	0.4778961947135649

0.2434251085946078	0.0255013208838602	0.4805812890359561
0.4962815476904366	0.7788296204597021	0.4774886669215394
0.9942431377817639	0.2759798104583784	0.4775819697763104
0.7452347535250516	0.5248152417297486	0.4833708429620898
0.9931325237872496	0.7768212460354318	0.4806391649689825
0.6364144808336263	0.3861856260832157	0.5296282556493007
0.7567850569735384	0.4385521422279662	0.5845196692898601

The structural information of *C

7.7705998421000002	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.7708997726000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.8873004912999995

Ta	Na	O	Rh	C
12	12	36	16	1

Direct

0.2505700000000033	0.7500000000000000	0.0000000000000000
0.2505700000000033	0.2500000000000000	0.0000000000000000
0.7505700000000033	0.2500000000000000	0.0000000000000000
0.7505700000000033	0.7500000000000000	0.0000000000000000
0.7501900000000035	0.2500000000000000	0.1373099999999994
0.2501900000000035	0.7500000000000000	0.1373099999999994
0.2501900000000035	0.2500000000000000	0.1373099999999994
0.7501900000000035	0.7500000000000000	0.1373099999999994
0.7491665365840900	0.2534252042950766	0.2769356784434904
0.2489444479057054	0.7532805062475479	0.2766954834051997
0.7520185954849011	0.7551603573003565	0.2764227131311729
0.2513381000644066	0.2528308648604934	0.2767247362185258
0.0003799999999998	0.5000000000000000	0.0686600000000013
0.0003799999999998	0.0000000000000000	0.0686600000000013
0.5003799999999998	0.0000000000000000	0.0686600000000013
0.5003799999999998	0.5000000000000000	0.0686600000000013
0.5000000000000000	0.0000000000000000	0.2059700000000007
0.0000000000000000	0.5000000000000000	0.2059700000000007
0.0000000000000000	0.0000000000000000	0.2059700000000007
0.5000000000000000	0.5000000000000000	0.2059700000000007
-0.0004134124556502	0.0192825822248868	0.3323972883738588

0.4984494135003149	0.5195737011009783	0.3320393683962473
0.0028541749620847	0.5088611684473098	0.3319810936810054
0.4988829991379078	0.0091047019624739	0.3323366994195627
0.2505700000000033	0.5000000000000000	0.0000000000000000
0.5005700000000033	0.7500000000000000	0.0000000000000000
0.0005700000000033	0.2500000000000000	0.0000000000000000
0.2505700000000033	0.0000000000000000	0.0000000000000000
0.5005700000000033	0.2500000000000000	0.0000000000000000
0.0005700000000033	0.7500000000000000	0.0000000000000000
0.7505700000000033	0.5000000000000000	0.0000000000000000
0.7505700000000033	0.0000000000000000	0.0000000000000000
0.7503799999999998	0.2500000000000000	0.0686600000000013
0.7503799999999998	0.7500000000000000	0.0686600000000013
0.2503799999999998	0.2500000000000000	0.0686600000000013
0.2503799999999998	0.7500000000000000	0.0686600000000013
0.5001900000000035	0.2500000000000000	0.1373099999999994
0.0001900000000035	0.2500000000000000	0.1373099999999994
0.7501900000000035	0.0000000000000000	0.1373099999999994
0.2501900000000035	0.5000000000000000	0.1373099999999994
0.5001900000000035	0.7500000000000000	0.1373099999999994
0.7501900000000035	0.5000000000000000	0.1373099999999994
0.2501900000000035	0.0000000000000000	0.1373099999999994
0.0001900000000035	0.7500000000000000	0.1373099999999994
0.2500000000000000	0.7500000000000000	0.2059700000000007
0.2500000000000000	0.2500000000000000	0.2059700000000007
0.7500000000000000	0.2500000000000000	0.2059700000000007
0.7500000000000000	0.7500000000000000	0.2059700000000007
0.5001839407840424	0.8017148783616397	0.2742632471192799
0.0003988746772226	0.3019250201438025	0.2744592097302802
0.8032157334326583	0.0015169093394696	0.2725235711215331
0.3013891940482077	0.5004254122441573	0.2736202250613737
0.7002027155564242	0.5013780834765054	0.2744614223933090
0.5004057072669108	0.1993581517134480	0.2727401041774457
0.0005252180524160	0.6988125951727742	0.2725237131383825
0.1986492921172631	0.0004761004776310	0.2734679826729795

0.7488472491366631	0.2391977251915629	0.3436937947030164
0.2519377586164539	0.2416369383758592	0.3435640527728708
0.2482789769413135	0.7435795658891469	0.3436219794638629
0.7537401619423469	0.7532506667516039	0.3431631632664674
0.5042396967316972	-0.0250733083450115	0.4251102582664082
0.2495174641637907	0.2282977397484791	0.4148286071697971
0.4960270184868242	0.4680130607729753	0.4244467435415509
-0.0036234700412897	-0.0280675513047445	0.4251643104111859
0.7496104082918923	0.2200728239094024	0.4150950829572094
0.2477338010021969	0.7265701548485408	0.4149068240985951
0.7463716743565668	0.6931282703886157	0.4117010833106228
0.0035356035437771	0.4728024028778408	0.4248350381387541
0.4963172261135285	0.2231950187503559	0.4809017985036331
0.2505026411100825	0.4726743284490579	0.4806827490458208
0.7505007650732420	-0.0096016865026164	0.4857817593683519
0.2505791515197985	-0.0227944848747168	0.4792548594838125
0.4904079543926775	0.7252663760950504	0.4826293718723126
0.0035178449460588	0.2234393892820596	0.4800140034449011
0.7500916386904817	0.4715198966122740	0.4820308235750077
0.0135019298180191	0.7264196026142766	0.4847323811970031
0.7538836814360971	0.7355441886912577	0.4812313115166258

The structural information of *CH

7.7705998421000002	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.7708997726000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.8873004912999995

Ta	Na	O	Rh	C	H
12	12	36	16	1	1

Direct

0.25057000000000033	0.7500000000000000	0.0000000000000000
0.25057000000000033	0.2500000000000000	0.0000000000000000
0.75057000000000033	0.2500000000000000	0.0000000000000000
0.75057000000000033	0.7500000000000000	0.0000000000000000
0.75019000000000035	0.2500000000000000	0.1373099999999994
0.25019000000000035	0.7500000000000000	0.1373099999999994
0.25019000000000035	0.2500000000000000	0.1373099999999994

0.75019000000000035	0.75000000000000000	0.13730999999999994
0.7486594556545887	0.2525938480874861	0.2767025521831534
0.2487318058004440	0.7526347843978186	0.2767179829922440
0.7513868947750728	0.7525896440079726	0.2759496655319779
0.2513554758729925	0.2525390725160563	0.2770629904045039
0.00037999999999998	0.50000000000000000	0.06866000000000013
0.00037999999999998	0.00000000000000000	0.06866000000000013
0.50037999999999998	0.00000000000000000	0.06866000000000013
0.50037999999999998	0.50000000000000000	0.06866000000000013
0.50000000000000000	0.00000000000000000	0.20597000000000007
0.00000000000000000	0.50000000000000000	0.20597000000000007
0.00000000000000000	0.00000000000000000	0.20597000000000007
0.50000000000000000	0.50000000000000000	0.20597000000000007
-0.0002866555138634	0.0191312432837696	0.3320323368285649
0.5001611219196631	0.5182383688032343	0.3320576029176979
0.0010535172442577	0.5083156397931758	0.3320142421009959
0.5000998801460678	0.0077796399914786	0.3320227499689090
0.25057000000000033	0.50000000000000000	0.00000000000000000
0.50057000000000033	0.75000000000000000	0.00000000000000000
0.00057000000000033	0.25000000000000000	0.00000000000000000
0.25057000000000033	0.00000000000000000	0.00000000000000000
0.50057000000000033	0.25000000000000000	0.00000000000000000
0.00057000000000033	0.75000000000000000	0.00000000000000000
0.75057000000000033	0.50000000000000000	0.00000000000000000
0.75057000000000033	0.00000000000000000	0.00000000000000000
0.75037999999999998	0.25000000000000000	0.06866000000000013
0.75037999999999998	0.75000000000000000	0.06866000000000013
0.25037999999999998	0.25000000000000000	0.06866000000000013
0.25037999999999998	0.75000000000000000	0.06866000000000013
0.50019000000000035	0.25000000000000000	0.13730999999999994
0.00019000000000035	0.25000000000000000	0.13730999999999994
0.75019000000000035	0.00000000000000000	0.13730999999999994
0.25019000000000035	0.50000000000000000	0.13730999999999994
0.50019000000000035	0.75000000000000000	0.13730999999999994
0.75019000000000035	0.50000000000000000	0.13730999999999994

0.25019000000000035	0.0000000000000000	0.13730999999999994
0.00019000000000035	0.7500000000000000	0.13730999999999994
0.25000000000000000	0.7500000000000000	0.20597000000000007
0.25000000000000000	0.2500000000000000	0.20597000000000007
0.75000000000000000	0.2500000000000000	0.20597000000000007
0.75000000000000000	0.7500000000000000	0.20597000000000007
0.4999950000321109	0.8007256547845520	0.2742195414133339
-0.0000339574098345	0.3004135024630583	0.2745757690316460
0.8015658531669240	0.0000105595778531	0.2732601396796263
0.3011715450526239	0.4999666928190102	0.2736908864426994
0.6984819542079417	0.4999664951819260	0.2733403223298566
0.4999332259336943	0.1981500025640340	0.2727250038754857
0.0000486516634335	0.6979485540865976	0.2724069225215535
0.1986704825849940	0.0000116650882235	0.2736533771661068
0.7474846205870600	0.2427381047292592	0.3435238739921379
0.2519943885505897	0.2430229173152234	0.3439331304515761
0.2476817169571906	0.7433280081557215	0.3435487985048928
0.7522542726480353	0.7434098820802801	0.3428798007882557
0.4980025453671532	-0.0227057072096711	0.4246979788244848
0.2498989908168077	0.2291551869169888	0.4160041828376526
0.4978190643729407	0.4743637145512820	0.4246512762821177
0.0008410747157456	-0.0226837995324782	0.4245410084565243
0.7494796460213232	0.2300743982766766	0.4146100045333021
0.2491894747045040	0.7281508447267854	0.4145989349067398
0.7493886296987267	0.7289985553813840	0.4120416167130583
0.0014002850950866	0.4744698987279216	0.4247415607683062
0.5030730573149146	0.2259228519550431	0.4801176622686517
0.2496682874335968	0.4824055562746428	0.4802373645882237
0.7494707970880548	-0.0309594019973830	0.4815290747040987
0.2493867995807896	-0.0248169278070356	0.4799837624821123
0.5082525750590192	0.7262382183079333	0.4815313215389137
-0.0039033741597166	0.2255861141206670	0.4800526399069014
0.7496534326184245	0.4861357753411459	0.4813886428047635
-0.0090253705752180	0.7267222715162225	0.4815131323498059
0.7496733852201786	0.7270221087109781	0.5144798213876569

0.7496036144043061 0.7269620529519752 0.5528125260589370

The structural information of *CH₂

7.7705998421000002	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.7708997726000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.8873004912999995

Ta	Na	O	Rh	C	H
12	12	36	16	1	2

Direct

0.2505699989999997	0.7500000000000000	0.0000000000000000
0.2505699989999997	0.2500000000000000	0.0000000000000000
0.7505699989999997	0.2500000000000000	0.0000000000000000
0.7505699989999997	0.7500000000000000	0.0000000000000000
0.7501900199999980	0.2500000000000000	0.1373099979999992
0.2501899900000026	0.7500000000000000	0.1373099979999992
0.2501899900000026	0.2500000000000000	0.1373099979999992
0.7501900199999980	0.7500000000000000	0.1373099979999992
0.7501642908846651	0.2499859457405695	0.2766632463222532
0.2502682236436150	0.7495225993612881	0.2766567673002213
0.7499480717711927	0.7494689539834234	0.2766789010576316
0.2500694198560736	0.2498127826472960	0.2766546178009439
0.0003799999999998	0.5000000000000000	0.0686599980000011
0.0003799999999998	0.0000000000000000	0.0686599980000011
0.5003799799999982	0.0000000000000000	0.0686599980000011
0.5003799799999982	0.5000000000000000	0.0686599980000011
0.5000000000000000	0.0000000000000000	0.2059700040000010
0.0000000000000000	0.5000000000000000	0.2059700040000010
0.0000000000000000	0.0000000000000000	0.2059700040000010
0.5000000000000000	0.5000000000000000	0.2059700040000010
-0.0021336905415979	0.9986022442962964	0.3319082217239442
0.4977798653103168	0.4986599973759766	0.3317924366671868
0.0027071863914846	0.4993347010005412	0.3318232065381443
0.5022361101074193	0.9993963087591134	0.3318223744512830
0.2505699989999997	0.5000000000000000	0.0000000000000000
0.5005699989999997	0.7500000000000000	0.0000000000000000
0.0005700000000033	0.2500000000000000	0.0000000000000000

0.2505699989999997	0.0000000000000000	0.0000000000000000
0.5005699989999997	0.2500000000000000	0.0000000000000000
0.0005700000000033	0.7500000000000000	0.0000000000000000
0.7505699989999997	0.5000000000000000	0.0000000000000000
0.7505699989999997	0.0000000000000000	0.0000000000000000
0.7503799799999982	0.2500000000000000	0.0686599980000011
0.7503799799999982	0.7500000000000000	0.0686599980000011
0.2503800089999970	0.2500000000000000	0.0686599980000011
0.2503800089999970	0.7500000000000000	0.0686599980000011
0.5001900199999980	0.2500000000000000	0.1373099979999992
0.0001900000000035	0.2500000000000000	0.1373099979999992
0.7501900199999980	0.0000000000000000	0.1373099979999992
0.2501899900000026	0.5000000000000000	0.1373099979999992
0.5001900199999980	0.7500000000000000	0.1373099979999992
0.7501900199999980	0.5000000000000000	0.1373099979999992
0.2501899900000026	0.0000000000000000	0.1373099979999992
0.0001900000000035	0.7500000000000000	0.1373099979999992
0.2500000000000000	0.7500000000000000	0.2059700040000010
0.2500000000000000	0.2500000000000000	0.2059700040000010
0.7500000000000000	0.2500000000000000	0.2059700040000010
0.7500000000000000	0.7500000000000000	0.2059700040000010
0.4999510480666686	0.8010675431869329	0.2734777709022789
-0.0000269636635675	0.3009342714434937	0.2733918495258525
0.8005070220671515	-0.0000858900444248	0.2734665975082257
0.3009882097997995	0.4998992470259841	0.2730351358056218
0.6982910358275026	0.4999191190287628	0.2735068002566514
0.4999824270152434	0.1987945293092874	0.2735786336132038
-0.0000339823953657	0.6989318749827452	0.2735148037598089
0.1989624919765990	-0.0001281786526783	0.2740581959656880
0.7506775412151422	0.2502873383051317	0.3435489651480919
0.2504570155161117	0.2543425153874687	0.3435828864854412
0.2506690789535855	0.7461222682527876	0.3435932159363481
0.7503625185794772	0.7505498276869648	0.3435550061930947
0.4940659140380946	0.0011475464116528	0.4247976890597358
0.2509207441155203	0.2457688838441258	0.4146658947801362

0.5080293145091423	0.5011645918595745	0.4246363299427517
0.0078420662634547	0.0010537421223603	0.4248324291675337
0.7509536735021139	0.2516948603662829	0.4145902020518525
0.2508555455059470	0.7565120599168506	0.4146761928838776
0.7509575842634311	0.7501361913515612	0.4146347848142740
-0.0059538978133884	0.5012895945059669	0.4246630227875789
0.5033167728176253	0.2499416098638638	0.4796612165668118
0.2510098916222824	0.5009883613858629	0.4764499583063742
0.7508221099063299	0.0011025918460789	0.4773651252473203
0.2510949143087154	0.0011686207654239	0.4821341941971550
0.5030883450618785	0.7523470644114103	0.4796760818618852
0.9985281956546601	0.2498164643187283	0.4796280445988394
0.7510603574024586	0.5012427802136730	0.4856161189527605
-0.0013649941917216	0.7525111583306398	0.4797506526537933
0.7519542893098393	0.5070059551823156	0.5499498170924403
0.7532113438657461	0.3884136888584593	0.5707009173897909
0.7512145478977140	0.6282188251945937	0.5695473100276703

The structural information of *CH₃

7.7705998421000002	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.7708997726000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.8873004912999995

Ta	Na	O	Rh	C	H
12	12	36	16	1	3

Direct

0.2505700000000033	0.7500000000000000	0.0000000000000000
0.2505700000000033	0.2500000000000000	0.0000000000000000
0.7505700000000033	0.2500000000000000	0.0000000000000000
0.7505700000000033	0.7500000000000000	0.0000000000000000
0.7501900000000035	0.2500000000000000	0.1373099999999994
0.2501900000000035	0.7500000000000000	0.1373099999999994
0.2501900000000035	0.2500000000000000	0.1373099999999994
0.7501900000000035	0.7500000000000000	0.1373099999999994
0.7508840529730111	0.2493289203082528	0.2766623640945181
0.2508022695110075	0.7491495108036921	0.2765825522968855
0.7511700918103854	0.7498016411380749	0.2766510467258405

0.2511113420064908	0.2500580432416870	0.2765746208431795
0.0003799999999998	0.5000000000000000	0.0686600000000013
0.0003799999999998	0.0000000000000000	0.0686600000000013
0.5003799999999998	0.0000000000000000	0.0686600000000013
0.5003799999999998	0.5000000000000000	0.0686600000000013
0.5000000000000000	0.0000000000000000	0.2059700000000007
0.0000000000000000	0.5000000000000000	0.2059700000000007
0.0000000000000000	0.0000000000000000	0.2059700000000007
0.5000000000000000	0.5000000000000000	0.2059700000000007
0.0047890479656951	0.9990483693339242	0.3315908348326504
0.5035730058574044	0.4990121971007151	0.3318652321991574
0.0039832738920253	0.4977362179645935	0.3318956771572889
0.5038602065955842	0.9977012697524059	0.3317037719905317
0.2505700000000033	0.5000000000000000	0.0000000000000000
0.5005700000000033	0.7500000000000000	0.0000000000000000
0.0005700000000033	0.2500000000000000	0.0000000000000000
0.2505700000000033	0.0000000000000000	0.0000000000000000
0.5005700000000033	0.2500000000000000	0.0000000000000000
0.0005700000000033	0.7500000000000000	0.0000000000000000
0.7505700000000033	0.5000000000000000	0.0000000000000000
0.7505700000000033	0.0000000000000000	0.0000000000000000
0.7503799999999998	0.2500000000000000	0.0686600000000013
0.7503799999999998	0.7500000000000000	0.0686600000000013
0.2503799999999998	0.2500000000000000	0.0686600000000013
0.2503799999999998	0.7500000000000000	0.0686600000000013
0.5001900000000035	0.2500000000000000	0.1373099999999994
0.0001900000000035	0.2500000000000000	0.1373099999999994
0.7501900000000035	0.0000000000000000	0.1373099999999994
0.2501900000000035	0.5000000000000000	0.1373099999999994
0.5001900000000035	0.7500000000000000	0.1373099999999994
0.7501900000000035	0.5000000000000000	0.1373099999999994
0.2501900000000035	0.0000000000000000	0.1373099999999994
0.0001900000000035	0.7500000000000000	0.1373099999999994
0.2500000000000000	0.7500000000000000	0.2059700000000007
0.2500000000000000	0.2500000000000000	0.2059700000000007

0.7500000000000000	0.2500000000000000	0.2059700000000007
0.7500000000000000	0.7500000000000000	0.2059700000000007
0.5002620867081192	0.6989242575567147	0.2735529473838593
0.0002624510409900	0.1989298964464788	0.2735241542383640
0.6994632545234196	-0.0000899542420041	0.2731228755682645
0.1991131947758712	0.4999214438258426	0.2730139679986538
0.8014687791627950	0.4998960817111446	0.2738434972894368
0.5002900489446059	0.3010359969733437	0.2733657522157880
0.0002554416570479	0.8010316472732563	0.2733303845691378
0.3010152060926320	-0.0000817845420826	0.2739365028869799
0.7478079432227543	0.2493121759612646	0.3435842051154193
0.2481109445955482	0.2530212396249927	0.3434828821923753
0.2476985896856850	0.7484751949023534	0.3434820488359788
0.7481890781322129	0.7520398585234014	0.3435697404722269
0.4873414614939945	0.0025565330405883	0.4243980823853110
0.2439032870565250	0.2507460088388049	0.4145115889538045
0.4972843497716321	0.5024826792058039	0.4247679137268242
-0.0015658030986372	0.0025040115884813	0.4243950262324093
0.7433645596739021	0.2552459887671855	0.4146370838458387
0.2438407280610739	0.7536242928478993	0.4145081474585627
0.7433909114347620	0.7491294293662341	0.4146157830781522
-0.0120553090934630	0.5025504238046206	0.4247097285067298
0.4952881604809484	0.2514451586551422	0.4796811587206400
0.2428893289242798	0.5022783832847970	0.4776129468481658
0.7428987260498855	0.0022402724381482	0.4774042973572912
0.2428687481975047	0.0022271282449121	0.4811119971492059
0.4953988299493901	0.7535460852769839	0.4796646827081097
-0.0084810342112762	0.2516916032937415	0.4795630650122541
0.7433853830060846	0.5022236927458464	0.4838151921608512
-0.0084889699209711	0.7533111254185142	0.4795762850645653
0.7504897072445421	0.5004837275307108	0.5557121959934148
0.8145843026662094	0.3821279862916946	0.5673392386000061
0.8202257270481832	0.6152730702813389	0.5675730027841733
0.6161700524444033	0.5035622482766378	0.5676401958476552

The structural information of *CH₄

7.7705998421000002	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.7708997726000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.8873004912999995

Ta	Na	O	Rh	C	H
12	12	36	16	1	4

Direct

0.2505700000000033	0.7500000000000000	0.0000000000000000
0.2505700000000033	0.2500000000000000	0.0000000000000000
0.7505700000000033	0.2500000000000000	0.0000000000000000
0.7505700000000033	0.7500000000000000	0.0000000000000000
0.7501900000000035	0.2500000000000000	0.1373099999999994
0.2501900000000035	0.7500000000000000	0.1373099999999994
0.2501900000000035	0.2500000000000000	0.1373099999999994
0.7501900000000035	0.7500000000000000	0.1373099999999994
0.7495567069131632	0.2513304737470435	0.2766712502696415
0.2495876193973920	0.7512368477773961	0.2766577611692474
0.7488714788851204	0.7504480709088094	0.2766746175034451
0.2488290797935492	0.2505320683861250	0.2766654792065509
0.0003799999999998	0.5000000000000000	0.0686600000000013
0.0003799999999998	0.0000000000000000	0.0686600000000013
0.5003799999999998	0.0000000000000000	0.0686600000000013
0.5003799999999998	0.5000000000000000	0.0686600000000013
0.5000000000000000	0.0000000000000000	0.2059700000000007
0.0000000000000000	0.5000000000000000	0.2059700000000007
0.0000000000000000	0.0000000000000000	0.2059700000000007
0.5000000000000000	0.5000000000000000	0.2059700000000007
-0.0055663100804429	0.0020460785763887	0.3317478862302567
0.4941502335867849	0.5020842687674831	0.3318384681002058
-0.0019446398814145	0.5053367974523372	0.3318424979182544
0.4978878712164930	0.0054929467580537	0.3317648197222441
0.2505700000000033	0.5000000000000000	0.0000000000000000
0.5005700000000033	0.7500000000000000	0.0000000000000000
0.0005700000000033	0.2500000000000000	0.0000000000000000
0.2505700000000033	0.0000000000000000	0.0000000000000000

0.5005700000000033	0.2500000000000000	0.0000000000000000
0.0005700000000033	0.7500000000000000	0.0000000000000000
0.7505700000000033	0.5000000000000000	0.0000000000000000
0.7505700000000033	0.0000000000000000	0.0000000000000000
0.7503799999999998	0.2500000000000000	0.0686600000000013
0.7503799999999998	0.7500000000000000	0.0686600000000013
0.2503799999999998	0.2500000000000000	0.0686600000000013
0.2503799999999998	0.7500000000000000	0.0686600000000013
0.5001900000000035	0.2500000000000000	0.1373099999999994
0.0001900000000035	0.2500000000000000	0.1373099999999994
0.7501900000000035	0.0000000000000000	0.1373099999999994
0.2501900000000035	0.5000000000000000	0.1373099999999994
0.5001900000000035	0.7500000000000000	0.1373099999999994
0.7501900000000035	0.5000000000000000	0.1373099999999994
0.2501900000000035	0.0000000000000000	0.1373099999999994
0.0001900000000035	0.7500000000000000	0.1373099999999994
0.2500000000000000	0.7500000000000000	0.2059700000000007
0.2500000000000000	0.2500000000000000	0.2059700000000007
0.7500000000000000	0.2500000000000000	0.2059700000000007
0.7500000000000000	0.7500000000000000	0.2059700000000007
0.4999985994560601	0.6989427755864919	0.2732763460412210
-0.0000175716112798	0.1989520136576247	0.2732688920716675
0.6993304751350701	0.0001502579533857	0.2737799844349383
0.1991540296094578	0.5001254056967245	0.2736735095650027
0.8013105108204278	0.5001847126231543	0.2732324085270448
0.5000043695666423	0.3009738324526680	0.2737222383975356
0.0000174644690216	0.8009749341790905	0.2737018773986531
0.3011529992189773	0.0001407022421143	0.2732614545933120
0.7522727628984778	0.2491471962024099	0.3435816641947798
0.2514313190083400	0.2482874368851228	0.3435523841648729
0.2522638040668146	0.7486220873593405	0.3435440705777457
0.7514950719617094	0.7478327568977987	0.3435881399635805
0.5063628350143211	-0.0053155299444709	0.4245431058898093
0.2554389128309780	0.2455064691527193	0.4147730975280214
0.5068483280041460	0.4948052759023703	0.4246741159947489

0.0063109609308377	-0.0051630596347946	0.4245684365998940
0.7555941693423850	0.2459466949295834	0.4147665196952393
0.2555625718606469	0.7454405562423201	0.4147660228897372
0.7554686665088994	0.7450045232364335	0.4147766550676527
0.0058864459696019	0.4947992682869812	0.4247215362338375
0.5054093654143073	0.2444319870221038	0.4796290644569587
0.2564503990086732	0.4953291917470443	0.4797774972626117
0.7563358385151694	-0.0046994747732857	0.4796822680020263
0.2562375114138147	-0.0045670747869005	0.4797501247684043
0.5053798769696062	0.7452085988548872	0.4796676245493452
0.0059109051648328	0.2445916961261541	0.4796476875727134
0.7560051140393277	0.4951556237900256	0.4802953127757540
0.0060227195046877	0.7452287026748563	0.4796184833505336
0.7672211890881979	0.5191748773671039	0.5980994286613295
0.6883138023731143	0.6331282581048090	0.5910238274540353
0.8402791033831427	0.4853264752608979	0.5666227535472502
0.8590080823464095	0.5468736350719298	0.6259921821917975
0.6844663084738449	0.4104934165357866	0.6075563615677444

The structural information of Ag@NaTaO₃

8.1117000580000003	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.1119003295999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.0289993286000012

Ta	Na	O	Ag
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12	12	36	16
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Direct

0.2509500000000031	0.5000000000000000	0.0000000000000000
0.2509500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.5000000000000000	0.0000000000000000
0.7505700000000033	0.0000000000000000	0.1366399999999999
0.2505700000000033	0.5000000000000000	0.1366399999999999
0.2505700000000033	0.0000000000000000	0.1366399999999999
0.7505700000000033	0.5000000000000000	0.1366399999999999
0.7507105604582155	0.0000000873685359	0.2755611989830319
0.2507105764215383	0.5000001124507456	0.2755616492794089

0.7507105595634813	0.4999999710361975	0.2755620948389752
0.2507106354720309	0.0000000259994433	0.2755605998414916
0.0007599999999996	0.7500000000000000	0.0683199999999999
0.0007599999999996	0.2500000000000000	0.0683199999999999
0.5007599999999996	0.2500000000000000	0.0683199999999999
0.5007599999999996	0.7500000000000000	0.0683199999999999
0.5003799999999998	0.2500000000000000	0.2049599999999998
0.0003799999999998	0.7500000000000000	0.2049599999999998
0.0003799999999998	0.2500000000000000	0.2049599999999998
0.5003799999999998	0.7500000000000000	0.2049599999999998
0.5004434185225485	0.2500014664113301	0.3234873377057115
0.0004440449432856	0.7499985723321425	0.3234873426047505
0.5004434122292701	0.7499986110427285	0.3234873346753847
0.0004440394553927	0.2500014921250847	0.3234873476437595
0.2509500000000031	0.7500000000000000	0.0000000000000000
0.2509500000000031	0.2500000000000000	0.0000000000000000
0.7509500000000031	0.7500000000000000	0.0000000000000000
0.0009500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.2500000000000000	0.0000000000000000
0.0009500000000031	0.5000000000000000	0.0000000000000000
0.5009500000000031	0.5000000000000000	0.0000000000000000
0.5009500000000031	0.0000000000000000	0.0000000000000000
0.7507599999999996	0.0000000000000000	0.0683199999999999
0.7507599999999996	0.5000000000000000	0.0683199999999999
0.2507599999999996	0.5000000000000000	0.0683199999999999
0.2507599999999996	0.0000000000000000	0.0683199999999999
0.0005700000000033	0.0000000000000000	0.1366399999999999
0.5005700000000033	0.0000000000000000	0.1366399999999999
0.7505700000000033	0.2500000000000000	0.1366399999999999
0.2505700000000033	0.7500000000000000	0.1366399999999999
0.5005700000000033	0.5000000000000000	0.1366399999999999
0.2505700000000033	0.2500000000000000	0.1366399999999999
0.7505700000000033	0.7500000000000000	0.1366399999999999
0.0005700000000033	0.5000000000000000	0.1366399999999999
0.2503799999999998	0.5000000000000000	0.2049599999999998

0.7503799999999998	0.5000000000000000	0.2049599999999998
0.2503799999999998	0.0000000000000000	0.2049599999999998
0.7503799999999998	0.0000000000000000	0.2049599999999998
0.7503368547983399	0.2499972799804617	0.2726624067904969
0.0003513950554365	0.5000000115906530	0.2726622327404457
0.0003514622139366	0.0000000070508668	0.2726616992379252
0.2503368525912804	0.2499972500077977	0.2726623576107307
0.7503368587853276	0.7500027262516739	0.2726623963287767
0.2503368506037374	0.7500027669576718	0.2726623647910065
0.5003534007604409	0.0000000122905461	0.2726616730259561
0.5003534018837399	0.5000000052256136	0.2726622244308342
0.7502768169186705	-0.0000000353497515	0.3406754077274966
0.2502769104221961	0.0000000109948444	0.3406758731569337
0.2502767877383243	0.4999999698563540	0.3406754552806985
0.7502768050997269	0.5000000229760313	0.3406750810082737
0.4998182485640540	0.2499996962681182	0.4251278667432754
0.2499361686863732	-0.0000000016308418	0.4169425533184149
0.4998182366481930	0.7500002636717032	0.4251278576585789
-0.0001817579547432	0.2499995482297694	0.4251278973391619
0.7499360847062315	-0.0000000146226306	0.4169426614961908
0.2499366210863475	0.4999999640056416	0.4169409592735080
0.7499367981535973	0.4999999801626588	0.4169410721113918
-0.0001817379850203	0.7500004095865562	0.4251278827028123
0.4999971311927409	-0.0000000240519245	0.4928134352518518
0.2499669448972799	0.7499974294689932	0.4928143761145971
0.7499668912089393	0.2499987301390991	0.4928143962319568
0.2499669332709288	0.2500025394612940	0.4928143894014410
0.4999979923940610	0.4999999901152465	0.4928139681871135
-0.0000027538085845	-0.0000000319692688	0.4928134877600923
0.7499668863909773	0.7500012332957973	0.4928143836579764
-0.0000017918860225	0.4999999946870414	0.4928139780816525

The structural information of *CO₂

8.1117000580000003	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.1119003295999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.0289993286000012

Ta	Na	O	Ag	C
12	12	38	16	1

Direct

0.2509500090000003	0.5000000000000000	0.0000000000000000
0.2509500090000003	0.0000000000000000	0.0000000000000000
0.7509499789999978	0.0000000000000000	0.0000000000000000
0.7509499789999978	0.5000000000000000	0.0000000000000000
0.7505699989999997	0.0000000000000000	0.1366399970000032
0.2505699989999997	0.5000000000000000	0.1366399970000032
0.2505699989999997	0.0000000000000000	0.1366399970000032
0.7505699989999997	0.5000000000000000	0.1366399970000032
0.7522556974787200	0.0022587611776888	0.2755580827591613
0.2522737139052538	0.5023044902186858	0.2754755120973545
0.7522720294562379	0.5022594099680333	0.2755204938308426
0.2522506748939143	0.0022906005660246	0.2755217781605924
0.0007599999999996	0.7500000000000000	0.0683199990000034
0.0007599999999996	0.2500000000000000	0.0683199990000034
0.5007600189999977	0.2500000000000000	0.0683199990000034
0.5007600189999977	0.7500000000000000	0.0683199990000034
0.5003799799999982	0.2500000000000000	0.2049600029999965
0.0003799999999998	0.7500000000000000	0.2049600029999965
0.0003799999999998	0.2500000000000000	0.2049600029999965
0.5003799799999982	0.7500000000000000	0.2049600029999965
0.5026627691929464	0.2530236286951881	0.3234574700435734
0.0028614674161152	0.7527139096057412	0.3234357659318067
0.5026316258031716	0.7527889766074282	0.3234503475681058
0.0027829406549486	0.2530109690115203	0.3234502250569612
0.2509500090000003	0.7500000000000000	0.0000000000000000
0.2509500090000003	0.2500000000000000	0.0000000000000000
0.7509499789999978	0.7500000000000000	0.0000000000000000
0.0009500000000003	0.0000000000000000	0.0000000000000000
0.7509499789999978	0.2500000000000000	0.0000000000000000
0.0009500000000003	0.5000000000000000	0.0000000000000000
0.5009499789999978	0.5000000000000000	0.0000000000000000
0.5009499789999978	0.0000000000000000	0.0000000000000000

0.7507600189999977	0.0000000000000000	0.0683199990000034
0.7507600189999977	0.5000000000000000	0.0683199990000034
0.2507599890000023	0.5000000000000000	0.0683199990000034
0.2507599890000023	0.0000000000000000	0.0683199990000034
0.00057000000000033	0.0000000000000000	0.1366399970000032
0.5005699989999997	0.0000000000000000	0.1366399970000032
0.7505699989999997	0.2500000000000000	0.1366399970000032
0.2505699989999997	0.7500000000000000	0.1366399970000032
0.5005699989999997	0.5000000000000000	0.1366399970000032
0.2505699989999997	0.2500000000000000	0.1366399970000032
0.7505699989999997	0.7500000000000000	0.1366399970000032
0.00057000000000033	0.5000000000000000	0.1366399970000032
0.2503800089999970	0.5000000000000000	0.2049600029999965
0.7503799799999982	0.5000000000000000	0.2049600029999965
0.2503800089999970	0.0000000000000000	0.2049600029999965
0.7503799799999982	0.0000000000000000	0.2049600029999965
0.7512259221824020	0.2505361209745919	0.2726585589378988
0.0008121864829605	0.5010912743289788	0.2726173918509526
0.0008118307184533	0.0010170724708637	0.2726760655189522
0.2512334684041541	0.2505271457709606	0.2726214632308718
0.7512057658951982	0.7506011960664503	0.2726942256886921
0.2512525093836817	0.7506074045674669	0.2726251527278858
0.5008663892772997	0.0010177775181624	0.2726903699850247
0.5008559303282845	0.5010491066547863	0.2726317731915922
0.7499803382417998	0.9996269740491045	0.3407103937113357
0.2499046309176899	0.9994653886368178	0.3406206659953496
0.2498603558980996	0.4994620863015291	0.3405409183393387
0.7499632161879133	0.4993796316529527	0.3406301628171040
0.7500030132986165	0.3573466800322338	0.6012985406191961
0.7497447806870413	0.6476923348264800	0.6013472473896450
0.4996124455300201	0.2495419962574321	0.4250472850675869
0.2499759408075575	0.0000085768788083	0.4168510608685743
0.4995237247953466	0.7501585457005654	0.4250258714729703
0.0000625881583411	0.2495682353765520	0.4250254465683912
0.7499626891595587	-0.0000219525895099	0.4169028063142770

0.2499922955608433	0.4999868869042512	0.4167021685934471
0.7499597769796326	0.5000022950146961	0.4168700015649230
0.0002151065588124	0.7501525811622146	0.4250067030861285
0.4999067484311593	-0.0000588190403022	0.4928403851874485
0.2499488210754509	0.7500465064690357	0.4928673091320510
0.7499001368822970	0.2502276417136534	0.4925480744596693
0.2499316622788035	0.2499080286193174	0.4928504636875188
0.4989065042351456	0.4999294890381364	0.4924412003235043
0.0000205499871113	-0.0000234409442766	0.4928062660813279
0.7499233212896631	0.7496444830559617	0.4924713062200483
0.0008876164243411	0.4999329311841674	0.4924293826303363
0.7498659529646867	0.5025171659126580	0.6011496813667672

The structural information of *COOH

8.1117000580000003	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.1119003295999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.0289993286000012

Ta	Na	O	Ag	C	H
12	12	38	16	1	1

Direct

0.2509500000000031	0.5000000000000000	0.0000000000000000
0.2509500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.5000000000000000	0.0000000000000000
0.7505700000000033	0.0000000000000000	0.1366399999999999
0.2505700000000033	0.5000000000000000	0.1366399999999999
0.2505700000000033	0.0000000000000000	0.1366399999999999
0.7505700000000033	0.5000000000000000	0.1366399999999999
0.7581176833748561	0.0081237834238664	0.2751320583630227
0.2565929974290550	0.5085219953391005	0.2753567011846306
0.7561132337789885	0.5079661111052199	0.2751126519556774
0.2564967012887341	0.0070888135767088	0.2752157771061104
0.0007599999999996	0.7500000000000000	0.0683199999999999
0.0007599999999996	0.2500000000000000	0.0683199999999999
0.5007599999999996	0.2500000000000000	0.0683199999999999
0.5007599999999996	0.7500000000000000	0.0683199999999999

0.5003799999999998	0.2500000000000000	0.2049599999999998
0.0003799999999998	0.7500000000000000	0.2049599999999998
0.0003799999999998	0.2500000000000000	0.2049599999999998
0.5003799999999998	0.7500000000000000	0.2049599999999998
0.5080296055800195	0.2655711599185616	0.3255051215327847
0.0093257180589027	0.7673039891711593	0.3266385466220812
0.5112596813171778	0.7541758150472007	0.3260264622490185
0.0108057442190803	0.2530594447053946	0.3256782936060265
0.2509500000000003	0.7500000000000000	0.0000000000000000
0.2509500000000003	0.2500000000000000	0.0000000000000000
0.7509500000000003	0.7500000000000000	0.0000000000000000
0.0009500000000003	0.0000000000000000	0.0000000000000000
0.7509500000000003	0.2500000000000000	0.0000000000000000
0.0009500000000003	0.5000000000000000	0.0000000000000000
0.5009500000000003	0.5000000000000000	0.0000000000000000
0.5009500000000003	0.0000000000000000	0.0000000000000000
0.7507599999999996	0.0000000000000000	0.0683199999999999
0.7507599999999996	0.5000000000000000	0.0683199999999999
0.2507599999999996	0.5000000000000000	0.0683199999999999
0.2507599999999996	0.0000000000000000	0.0683199999999999
0.0005700000000003	0.0000000000000000	0.1366399999999999
0.5005700000000003	0.0000000000000000	0.1366399999999999
0.7505700000000003	0.2500000000000000	0.1366399999999999
0.2505700000000003	0.7500000000000000	0.1366399999999999
0.5005700000000003	0.5000000000000000	0.1366399999999999
0.2505700000000003	0.2500000000000000	0.1366399999999999
0.7505700000000003	0.7500000000000000	0.1366399999999999
0.0005700000000003	0.5000000000000000	0.1366399999999999
0.2503799999999998	0.5000000000000000	0.2049599999999998
0.7503799999999998	0.5000000000000000	0.2049599999999998
0.2503799999999998	0.0000000000000000	0.2049599999999998
0.7503799999999998	0.0000000000000000	0.2049599999999998
0.7409213985698048	0.2520542130729662	0.2729730375805797
0.0009692448606899	0.4914908627568262	0.2741957281188256
0.0013761050524838	0.0158279457647655	0.2701669802120417

0.2633788252219743	0.2517417523640305	0.2733595197281896
0.7633910933305871	0.7517715861666306	0.2720731588217904
0.2408142762738637	0.7515911525166913	0.2718969148676855
0.5013510731836467	0.9925963219590440	0.2745984362430166
0.5008044762253648	0.5141318522349331	0.2710683566987638
0.7638863020075756	0.9954947787812625	0.3402367670095942
0.2326905696012659	0.9939719528531071	0.3400288246994990
0.2577533326380574	0.5021014103388080	0.3407126578566168
0.7356648074797583	0.5024836766812377	0.3401934638135389
0.1361472959970031	0.6116430697682645	0.5744210622588775
0.9353614548117435	0.4644632340932703	0.6054528314839368
0.5080172498922799	0.2216142399066732	0.4299928188754912
0.2446412253553466	0.9939862717135047	0.4150744649425780
0.4964495865568854	0.7520319763658404	0.4333224351375567
0.9929612349962129	0.2479630831363710	0.4333093988711301
0.7644043717022563	0.9795266066457855	0.4147705349497435
0.2585724518552456	0.4898936375136470	0.4151739860185862
0.7599857326986816	0.4968779934811623	0.4136992102746223
0.0087099115735079	0.7302240473470263	0.4358409535179204
0.4267236120176469	0.9927964833987838	0.5011732875943100
0.2633409577259068	0.6724174827675020	0.5004994618420029
0.7413343418212589	0.1607329111412026	0.4998043714431267
0.2546273431531216	0.2988439338159103	0.4953918026242629
0.5592371450020488	0.4797760335400587	0.4932739885262717
0.0636218083549474	0.9941718381655433	0.4975598231923669
0.7430078057524171	0.8073265884698095	0.4988981703936619
0.9090670616588326	0.4840017782298920	0.5001755482616930
0.0115857472905580	0.5274675715762106	0.5674039098754197
0.8402077588635605	0.4014937613770838	0.5944882112104155

The structural information of *CO

8.1117000580000003	0.0000000000000000	0.0000000000000000		
0.0000000000000000	8.1119003295999992	0.0000000000000000		
0.0000000000000000	0.0000000000000000	29.0289993286000012		
Ta	Na	O	Ag	C
12	12	37	16	1

Direct

0.2509500000000031	0.5000000000000000	0.0000000000000000
0.2509500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.5000000000000000	0.0000000000000000
0.7505700000000033	0.0000000000000000	0.1366399999999999
0.2505700000000033	0.5000000000000000	0.1366399999999999
0.2505700000000033	0.0000000000000000	0.1366399999999999
0.7505700000000033	0.5000000000000000	0.1366399999999999
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0.2510444226904522	0.5000578504887815	0.2755883905813565
0.7524188298040494	0.5000337186941456	0.2755852001842398
0.2513614313766570	0.0000618513033735	0.2754035101716992
0.0007599999999996	0.7500000000000000	0.0683199999999999
0.0007599999999996	0.2500000000000000	0.0683199999999999
0.5007599999999996	0.2500000000000000	0.0683199999999999
0.5007599999999996	0.7500000000000000	0.0683199999999999
0.5003799999999998	0.2500000000000000	0.2049599999999998
0.0003799999999998	0.7500000000000000	0.2049599999999998
0.0003799999999998	0.2500000000000000	0.2049599999999998
0.5003799999999998	0.7500000000000000	0.2049599999999998
0.5019209132089817	0.2488704523672981	0.3230167804463597
0.0020214565068444	0.7493341363788827	0.3237932321396906
0.5019165202835959	0.7511966806006189	0.3230147854052979
0.0020213845547690	0.2507669648687837	0.3238039960173778
0.2509500000000031	0.7500000000000000	0.0000000000000000
0.2509500000000031	0.2500000000000000	0.0000000000000000
0.7509500000000031	0.7500000000000000	0.0000000000000000
0.0009500000000031	0.0000000000000000	0.0000000000000000
0.7509500000000031	0.2500000000000000	0.0000000000000000
0.0009500000000031	0.5000000000000000	0.0000000000000000
0.5009500000000031	0.5000000000000000	0.0000000000000000
0.5009500000000031	0.0000000000000000	0.0000000000000000
0.7507599999999996	0.0000000000000000	0.0683199999999999
0.7507599999999996	0.5000000000000000	0.0683199999999999

0.2507599999999996	0.5000000000000000	0.0683199999999999
0.2507599999999996	0.0000000000000000	0.0683199999999999
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0.50057000000000033	0.0000000000000000	0.1366399999999999
0.75057000000000033	0.2500000000000000	0.1366399999999999
0.25057000000000033	0.7500000000000000	0.1366399999999999
0.50057000000000033	0.5000000000000000	0.1366399999999999
0.25057000000000033	0.2500000000000000	0.1366399999999999
0.75057000000000033	0.7500000000000000	0.1366399999999999
0.00057000000000033	0.5000000000000000	0.1366399999999999
0.25037999999999998	0.5000000000000000	0.20495999999999998
0.75037999999999998	0.5000000000000000	0.20495999999999998
0.25037999999999998	0.0000000000000000	0.20495999999999998
0.75037999999999998	0.0000000000000000	0.20495999999999998
0.7501293764241347	0.2501147919530962	0.2726801494103692
0.0006246430877313	0.5000229214338204	0.2715137419924379
0.0005782121311765	0.0000107575618618	0.2721080235805735
0.2515041869801768	0.2501147009096165	0.2726795823816365
0.7501292489149541	0.7499046497093637	0.2726906001637829
0.2515054862457420	0.7499067406333765	0.2726887761695197
0.5005603327725330	0.0000122407766284	0.2729576291575271
0.5006108800931601	0.5000188286709201	0.2739814024547867
0.7526748772293110	0.0000267077151443	0.3405102608954923
0.2470618551796817	0.0000216447716608	0.3405025769703651
0.2415626858978642	0.4999697148369060	0.3407196425691563
0.7585876294812727	0.4999628819993044	0.3407418689362326
0.9926366681693893	0.5029284401625870	0.6051675912883069
0.4994465217812499	0.2523838366012258	0.4236456082785745
0.2488112371400449	0.0000186014343949	0.4166076666175898
0.4994267472966366	0.7476393799084124	0.4236354854165991
0.9995044940549810	0.2508117828121192	0.4264909790216058
0.7504515743465707	0.0000197774875311	0.4165977188062151
0.2459219022170394	0.5000312703550716	0.4169177931214907
0.7528997006641094	0.5000196591422809	0.4169025593676652
0.9995206376226938	0.7492626924202916	0.4264745921426559

0.4994741279116360	0.0000298562726502	0.4917276898106502
0.2553237490316396	0.7543514626288577	0.4925012768307823
0.7438546463583188	0.2454498475749697	0.4924710766415034
0.2553165015319522	0.2457767267107681	0.4925093620168501
0.4997229536510060	0.5000312716853458	0.4918857595375247
-0.0001265579178616	0.0000444185908466	0.4925475064218885
0.7438402806381514	0.7546276250134107	0.4924619865623081
-0.0001398452416371	0.5000155650693077	0.4935399234539540
0.9957474439694298	0.5017303066195540	0.5654357238833128